Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 10:46 AM EDT

PDB ID	:	3URO
Title	:	Poliovirus receptor CD155 D1D2
Authors	:	Zhang, P.; Mueller, S.; Morais, M.C.; Bator, C.M.; Bowman, V.D.; Hafenstein, S.; Wimmer, E.; Rossmann, M.G.
Deposited on	:	2011-11-22
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

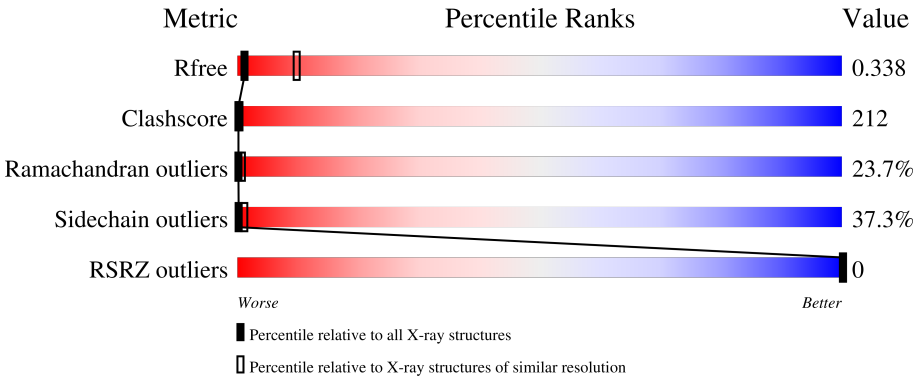
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	221	. 43% 40% 9% .

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1638 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Poliovirus receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	213	Total	C	N	O	S	0	0	0
			1638	1038	281	310	9			

There are 11 discrepancies between the modelled and reference sequences:

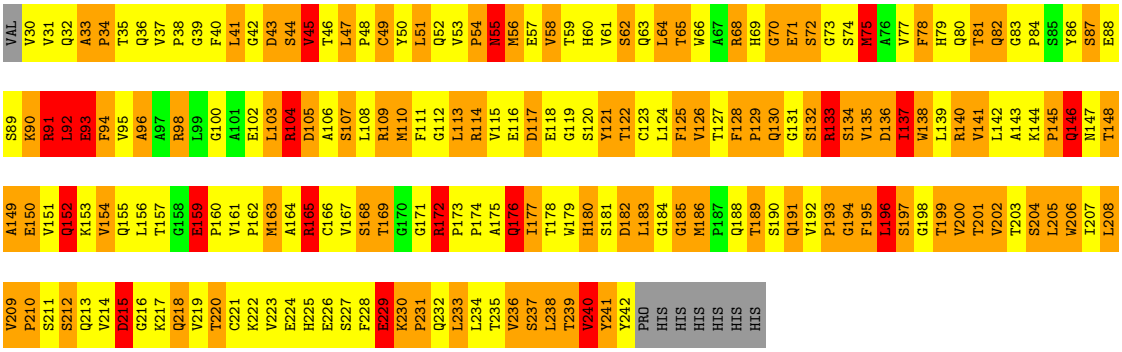
Chain	Residue	Modelled	Actual	Comment	Reference
R	105	ASP	ASN	ENGINEERED MUTATION	UNP P15151
R	120	SER	ASN	ENGINEERED MUTATION	UNP P15151
R	188	GLN	ASN	ENGINEERED MUTATION	UNP P15151
R	218	GLN	ASN	ENGINEERED MUTATION	UNP P15151
R	237	SER	ASN	ENGINEERED MUTATION	UNP P15151
R	244	HIS	-	EXPRESSION TAG	UNP P15151
R	245	HIS	-	EXPRESSION TAG	UNP P15151
R	246	HIS	-	EXPRESSION TAG	UNP P15151
R	247	HIS	-	EXPRESSION TAG	UNP P15151
R	248	HIS	-	EXPRESSION TAG	UNP P15151
R	249	HIS	-	EXPRESSION TAG	UNP P15151

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Poliovirus receptor

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	84.31Å 84.31Å 117.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.89 – 3.50 35.89 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (35.89-3.50) 99.3 (35.89-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.305 , 0.341 0.304 , 0.338	Depositor DCC
R_{free} test set	277 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	126.4	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 245.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	1638	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	R	0.56	0/1678	1.16	13/2289 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	R	0	2

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	92	LEU	CB-CA-C	15.51	139.68	110.20
1	R	93	GLU	N-CA-CB	12.02	132.24	110.60
1	R	92	LEU	N-CA-C	-8.53	87.96	111.00
1	R	91	ARG	CB-CA-C	7.60	125.60	110.40
1	R	146	GLN	N-CA-C	-6.72	92.87	111.00
1	R	220	THR	N-CA-CB	-6.14	98.63	110.30
1	R	152	GLN	N-CA-C	-6.13	94.46	111.00
1	R	121	TYR	CB-CA-C	-6.09	98.22	110.40
1	R	107	SER	N-CA-C	-5.96	94.90	111.00
1	R	141	VAL	N-CA-C	5.87	126.85	111.00
1	R	165	ARG	N-CA-C	-5.75	95.48	111.00
1	R	55	ASN	N-CA-C	-5.63	95.79	111.00
1	R	176	GLN	N-CA-C	-5.13	97.14	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	R	140	ARG	Peptide
1	R	45	VAL	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	1638	0	1620	692	0
All	All	1638	0	1620	692	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 212.

All (692) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:122:THR:CB	1:R:136:ASP:HA	1.70	1.19
1:R:36:GLN:HA	1:R:139:LEU:CG	1.73	1.16
1:R:122:THR:HB	1:R:136:ASP:CA	1.74	1.15
1:R:144:LYS:HE2	1:R:145:PRO:O	1.45	1.15
1:R:59:THR:HG21	1:R:129:PRO:HG2	1.21	1.12
1:R:214:VAL:HG13	1:R:214:VAL:O	1.41	1.12
1:R:124:LEU:HA	1:R:134:SER:OG	1.48	1.11
1:R:181:SER:HB3	1:R:219:VAL:HG23	1.25	1.11
1:R:114:ARG:HH21	1:R:115:VAL:HB	1.06	1.10
1:R:138:TRP:O	1:R:139:LEU:HD22	1.50	1.09
1:R:164:ALA:O	1:R:206:TRP:HB3	1.49	1.09
1:R:41:LEU:HD13	1:R:42:GLY:H	1.12	1.07
1:R:120:SER:HA	1:R:138:TRP:CD1	1.90	1.07
1:R:38:PRO:N	1:R:140:ARG:HB2	1.71	1.05
1:R:215:ASP:O	1:R:238:LEU:HB2	1.57	1.05
1:R:36:GLN:CA	1:R:139:LEU:HG	1.86	1.04
1:R:215:ASP:CB	1:R:216:GLY:HA3	1.87	1.04
1:R:155:GLN:CD	1:R:211:SER:HA	1.77	1.03
1:R:161:VAL:C	1:R:163:MET:HB3	1.77	1.03
1:R:43:ASP:HB2	1:R:44:SER:HA	1.34	1.03
1:R:59:THR:CG2	1:R:129:PRO:HG2	1.88	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:172:ARG:HB3	1:R:173:PRO:HD3	1.39	1.03
1:R:114:ARG:NH2	1:R:115:VAL:HB	1.74	1.01
1:R:194:GLY:HA3	1:R:201:THR:O	1.61	1.01
1:R:171:GLY:O	1:R:201:THR:HG22	1.60	1.01
1:R:215:ASP:HB3	1:R:240:VAL:HG22	1.42	1.01
1:R:68:ARG:HG2	1:R:69:HIS:H	1.25	1.00
1:R:222:LYS:HA	1:R:233:LEU:HB3	1.38	1.00
1:R:95:VAL:HG23	1:R:107:SER:O	1.61	0.99
1:R:40:PHE:O	1:R:43:ASP:HB3	1.62	0.99
1:R:63:GLN:HB3	1:R:79:HIS:HE1	1.21	0.99
1:R:201:THR:HG23	1:R:202:VAL:H	1.24	0.99
1:R:228:PHE:O	1:R:230:LYS:N	1.94	0.98
1:R:196:LEU:HD13	1:R:196:LEU:N	1.76	0.98
1:R:225:HIS:HB3	1:R:228:PHE:CZ	1.99	0.97
1:R:31:VAL:HA	1:R:51:LEU:HD21	1.47	0.97
1:R:63:GLN:HB3	1:R:79:HIS:CE1	2.00	0.97
1:R:65:THR:HA	1:R:78:PHE:O	1.66	0.96
1:R:75:MET:HG2	1:R:77:VAL:HB	1.44	0.96
1:R:204:SER:HB2	1:R:206:TRP:HE1	1.28	0.95
1:R:31:VAL:HG21	1:R:134:SER:HA	1.48	0.95
1:R:196:LEU:HB3	1:R:200:VAL:N	1.82	0.93
1:R:215:ASP:HB2	1:R:216:GLY:HA3	1.46	0.93
1:R:136:ASP:O	1:R:137:ILE:HB	1.69	0.93
1:R:37:VAL:H	1:R:139:LEU:HB3	1.34	0.93
1:R:46:THR:HB	1:R:109:ARG:HA	1.49	0.93
1:R:122:THR:HB	1:R:136:ASP:HA	0.93	0.93
1:R:31:VAL:HG23	1:R:133:ARG:HH21	1.34	0.92
1:R:37:VAL:N	1:R:139:LEU:HB3	1.85	0.92
1:R:118:GLU:HB3	1:R:138:TRP:HB2	1.49	0.92
1:R:214:VAL:O	1:R:214:VAL:CG1	2.14	0.91
1:R:71:GLU:O	1:R:73:GLY:N	2.04	0.91
1:R:192:VAL:CG1	1:R:204:SER:H	1.84	0.91
1:R:120:SER:HA	1:R:138:TRP:CG	2.06	0.90
1:R:121:TYR:O	1:R:137:ILE:N	2.04	0.90
1:R:155:GLN:OE1	1:R:211:SER:HA	1.71	0.90
1:R:144:LYS:HE2	1:R:145:PRO:C	1.91	0.89
1:R:41:LEU:CD1	1:R:42:GLY:H	1.86	0.89
1:R:44:SER:OG	1:R:112:GLY:HA3	1.71	0.89
1:R:86:TYR:CZ	1:R:94:PHE:CE2	2.60	0.89
1:R:36:GLN:HA	1:R:139:LEU:HG	0.92	0.89
1:R:196:LEU:HB3	1:R:200:VAL:H	1.35	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:132:SER:O	1:R:133:ARG:HB3	1.72	0.88
1:R:186:MET:SD	1:R:207:ILE:HB	2.14	0.88
1:R:186:MET:SD	1:R:209:VAL:HG22	2.14	0.88
1:R:89:SER:HA	1:R:91:ARG:NH2	1.89	0.88
1:R:59:THR:HG21	1:R:129:PRO:CG	2.04	0.87
1:R:95:VAL:CG2	1:R:107:SER:O	2.22	0.86
1:R:186:MET:C	1:R:188:GLN:H	1.77	0.86
1:R:204:SER:CB	1:R:206:TRP:HE1	1.89	0.86
1:R:214:VAL:HG22	1:R:217:LYS:HB2	1.57	0.86
1:R:124:LEU:C	1:R:125:PHE:HD1	1.79	0.85
1:R:215:ASP:CG	1:R:216:GLY:HA3	1.95	0.85
1:R:54:PRO:HA	1:R:55:ASN:HB2	1.58	0.85
1:R:144:LYS:HE3	1:R:145:PRO:HD2	1.59	0.85
1:R:41:LEU:HD13	1:R:42:GLY:N	1.92	0.85
1:R:93:GLU:HG3	1:R:111:PHE:CZ	2.12	0.85
1:R:145:PRO:HB3	1:R:171:GLY:N	1.92	0.85
1:R:189:THR:HA	1:R:208:LEU:HD13	1.59	0.84
1:R:206:TRP:N	1:R:206:TRP:CD2	2.44	0.84
1:R:228:PHE:O	1:R:228:PHE:CD2	2.29	0.84
1:R:152:GLN:O	1:R:163:MET:HG2	1.76	0.84
1:R:64:LEU:O	1:R:79:HIS:HA	1.78	0.83
1:R:69:HIS:HA	1:R:70:GLY:O	1.79	0.83
1:R:183:LEU:HD13	1:R:185:GLY:H	1.44	0.83
1:R:186:MET:SD	1:R:207:ILE:HD12	2.19	0.82
1:R:45:VAL:HG12	1:R:109:ARG:HH22	1.45	0.82
1:R:117:ASP:HB2	1:R:141:VAL:HB	1.61	0.81
1:R:86:TYR:CE1	1:R:94:PHE:CE2	2.68	0.81
1:R:41:LEU:H	1:R:143:ALA:HB2	1.45	0.81
1:R:179:TRP:CZ2	1:R:206:TRP:HA	2.15	0.80
1:R:38:PRO:HD3	1:R:140:ARG:HD2	1.61	0.80
1:R:90:LYS:H	1:R:90:LYS:HZ3	1.26	0.80
1:R:205:LEU:HA	1:R:206:TRP:CE2	2.17	0.80
1:R:81:THR:O	1:R:98:ARG:CZ	2.30	0.79
1:R:190:SER:O	1:R:205:LEU:HG	1.83	0.79
1:R:215:ASP:HB2	1:R:216:GLY:CA	2.13	0.79
1:R:160:PRO:HA	1:R:209:VAL:O	1.83	0.79
1:R:205:LEU:C	1:R:206:TRP:CG	2.56	0.78
1:R:111:PHE:CD2	1:R:111:PHE:O	2.36	0.78
1:R:145:PRO:HB3	1:R:171:GLY:H	1.45	0.78
1:R:149:ALA:HA	1:R:165:ARG:O	1.84	0.78
1:R:195:PHE:C	1:R:196:LEU:HD22	2.04	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:237:SER:O	1:R:238:LEU:HD13	1.84	0.77
1:R:43:ASP:HB2	1:R:44:SER:CA	2.13	0.77
1:R:138:TRP:C	1:R:139:LEU:HD22	2.04	0.77
1:R:123:CYS:O	1:R:134:SER:OG	2.03	0.77
1:R:123:CYS:O	1:R:124:LEU:HD13	1.85	0.77
1:R:172:ARG:NH1	1:R:173:PRO:HA	2.00	0.77
1:R:117:ASP:CB	1:R:141:VAL:HB	2.14	0.76
1:R:68:ARG:HG2	1:R:69:HIS:N	2.00	0.76
1:R:68:ARG:HD3	1:R:72:SER:HA	1.67	0.76
1:R:142:LEU:HB3	1:R:172:ARG:HG3	1.65	0.76
1:R:91:ARG:HG2	1:R:92:LEU:H	1.51	0.76
1:R:154:VAL:HA	1:R:241:TYR:CD2	2.20	0.75
1:R:213:GLN:O	1:R:214:VAL:HG12	1.87	0.75
1:R:63:GLN:CB	1:R:79:HIS:HE1	1.99	0.75
1:R:69:HIS:N	1:R:70:GLY:HA3	2.00	0.75
1:R:104:ARG:H	1:R:104:ARG:HD3	1.50	0.75
1:R:161:VAL:H	1:R:208:LEU:HA	1.51	0.75
1:R:224:GLU:O	1:R:225:HIS:HB2	1.87	0.74
1:R:60:HIS:CE1	1:R:104:ARG:HH22	2.05	0.74
1:R:49:CYS:O	1:R:49:CYS:SG	2.45	0.74
1:R:172:ARG:HB3	1:R:173:PRO:CD	2.16	0.74
1:R:41:LEU:HD22	1:R:43:ASP:OD2	1.88	0.74
1:R:78:PHE:HD1	1:R:79:HIS:N	1.86	0.74
1:R:196:LEU:N	1:R:196:LEU:CD1	2.50	0.74
1:R:172:ARG:HD3	1:R:173:PRO:CD	2.17	0.73
1:R:215:ASP:HB3	1:R:240:VAL:CG2	2.17	0.73
1:R:68:ARG:CG	1:R:69:HIS:H	2.00	0.73
1:R:143:ALA:O	1:R:172:ARG:HB3	1.89	0.73
1:R:216:GLY:H	1:R:238:LEU:H	1.36	0.73
1:R:159:GLU:OE2	1:R:160:PRO:HG3	1.88	0.73
1:R:38:PRO:CA	1:R:140:ARG:HB2	2.19	0.73
1:R:59:THR:CB	1:R:129:PRO:HG2	2.18	0.73
1:R:133:ARG:HD3	1:R:133:ARG:N	2.02	0.72
1:R:185:GLY:C	1:R:186:MET:HG3	2.07	0.72
1:R:199:THR:HG22	1:R:199:THR:O	1.90	0.72
1:R:102:GLU:HB2	1:R:104:ARG:N	2.04	0.72
1:R:56:MET:SD	1:R:56:MET:N	2.61	0.72
1:R:142:LEU:HD13	1:R:172:ARG:HG3	1.72	0.72
1:R:154:VAL:HG23	1:R:155:GLN:N	2.04	0.72
1:R:186:MET:HE2	1:R:209:VAL:HG13	1.69	0.72
1:R:228:PHE:O	1:R:228:PHE:HD2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:43:ASP:CB	1:R:44:SER:HA	2.18	0.72
1:R:86:TYR:CZ	1:R:94:PHE:CD2	2.78	0.72
1:R:183:LEU:HD13	1:R:185:GLY:N	2.05	0.72
1:R:45:VAL:O	1:R:110:MET:O	2.07	0.71
1:R:93:GLU:HG3	1:R:111:PHE:CE1	2.24	0.71
1:R:80:GLN:HA	1:R:83:GLY:O	1.90	0.71
1:R:118:GLU:HB2	1:R:138:TRP:CE3	2.24	0.71
1:R:196:LEU:H	1:R:202:VAL:HG12	1.56	0.71
1:R:201:THR:HG23	1:R:202:VAL:N	2.04	0.71
1:R:75:MET:CG	1:R:77:VAL:HB	2.17	0.71
1:R:149:ALA:CB	1:R:166:CYS:HA	2.20	0.71
1:R:199:THR:O	1:R:200:VAL:HG13	1.91	0.71
1:R:206:TRP:HE3	1:R:206:TRP:O	1.73	0.71
1:R:146:GLN:O	1:R:146:GLN:HG3	1.90	0.71
1:R:44:SER:OG	1:R:111:PHE:HA	1.91	0.71
1:R:69:HIS:N	1:R:70:GLY:CA	2.54	0.70
1:R:64:LEU:HD11	1:R:106:ALA:HB3	1.73	0.70
1:R:221:CYS:O	1:R:233:LEU:CB	2.40	0.70
1:R:135:VAL:HG13	1:R:136:ASP:O	1.90	0.70
1:R:118:GLU:OE2	1:R:141:VAL:HG12	1.91	0.70
1:R:191:GLN:HA	1:R:205:LEU:HG	1.74	0.70
1:R:222:LYS:HE2	1:R:231:PRO:HB2	1.72	0.70
1:R:125:PHE:CD1	1:R:125:PHE:N	2.58	0.70
1:R:179:TRP:CD2	1:R:207:ILE:HG23	2.26	0.70
1:R:225:HIS:HB3	1:R:228:PHE:CE1	2.27	0.70
1:R:159:GLU:CD	1:R:160:PRO:HD3	2.11	0.69
1:R:35:THR:O	1:R:36:GLN:CD	2.30	0.69
1:R:52:GLN:O	1:R:54:PRO:HD3	1.91	0.69
1:R:149:ALA:HB2	1:R:166:CYS:HA	1.74	0.69
1:R:217:LYS:NZ	1:R:218:GLN:HE21	1.91	0.69
1:R:221:CYS:O	1:R:233:LEU:HB2	1.92	0.69
1:R:53:VAL:HG12	1:R:55:ASN:HA	1.73	0.69
1:R:86:TYR:OH	1:R:94:PHE:CD2	2.45	0.69
1:R:47:LEU:HD11	1:R:108:LEU:HB2	1.74	0.69
1:R:78:PHE:CE1	1:R:80:GLN:HB2	2.28	0.69
1:R:104:ARG:HD3	1:R:104:ARG:N	2.07	0.69
1:R:121:TYR:H	1:R:138:TRP:HB3	1.58	0.69
1:R:209:VAL:HG12	1:R:210:PRO:HD2	1.75	0.69
1:R:45:VAL:HA	1:R:109:ARG:NH1	2.08	0.69
1:R:89:SER:HA	1:R:91:ARG:HH22	1.55	0.69
1:R:177:ILE:HG22	1:R:222:LYS:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:196:LEU:HA	1:R:200:VAL:O	1.94	0.68
1:R:66:TRP:HA	1:R:122:THR:O	1.92	0.68
1:R:121:TYR:O	1:R:137:ILE:O	2.11	0.68
1:R:225:HIS:HB3	1:R:228:PHE:HZ	1.57	0.68
1:R:41:LEU:HD11	1:R:113:LEU:O	1.93	0.68
1:R:240:VAL:O	1:R:241:TYR:CD2	2.46	0.68
1:R:192:VAL:HG12	1:R:204:SER:H	1.59	0.68
1:R:44:SER:CB	1:R:113:LEU:HD23	2.24	0.68
1:R:45:VAL:N	1:R:110:MET:O	2.27	0.68
1:R:229:GLU:HG3	1:R:230:LYS:N	2.09	0.67
1:R:60:HIS:HB3	1:R:61:VAL:CG1	2.24	0.67
1:R:164:ALA:O	1:R:206:TRP:CB	2.34	0.67
1:R:68:ARG:HB2	1:R:70:GLY:HA3	1.76	0.67
1:R:215:ASP:CA	1:R:240:VAL:HG13	2.25	0.67
1:R:217:LYS:H	1:R:238:LEU:HD23	1.58	0.67
1:R:144:LYS:C	1:R:171:GLY:HA2	2.14	0.67
1:R:118:GLU:CB	1:R:138:TRP:CE3	2.77	0.67
1:R:195:PHE:O	1:R:196:LEU:HD22	1.93	0.67
1:R:60:HIS:CB	1:R:61:VAL:HA	2.24	0.67
1:R:94:PHE:HA	1:R:108:LEU:HD13	1.77	0.66
1:R:172:ARG:CB	1:R:173:PRO:HD3	2.22	0.66
1:R:192:VAL:HG12	1:R:204:SER:O	1.96	0.66
1:R:68:ARG:H	1:R:68:ARG:HD2	1.60	0.66
1:R:181:SER:OG	1:R:186:MET:HE3	1.94	0.66
1:R:219:VAL:O	1:R:235:THR:HG22	1.96	0.66
1:R:118:GLU:OE2	1:R:139:LEU:O	2.13	0.66
1:R:189:THR:HB	1:R:207:ILE:HG22	1.77	0.66
1:R:183:LEU:HD13	1:R:185:GLY:HA3	1.76	0.66
1:R:217:LYS:H	1:R:238:LEU:CD2	2.09	0.65
1:R:55:ASN:H	1:R:57:GLU:H	1.44	0.65
1:R:152:GLN:HB2	1:R:153:LYS:HG2	1.79	0.65
1:R:33:ALA:CB	1:R:49:CYS:HA	2.26	0.65
1:R:87:SER:C	1:R:89:SER:H	1.99	0.65
1:R:142:LEU:CD1	1:R:172:ARG:HG3	2.26	0.65
1:R:216:GLY:H	1:R:238:LEU:N	1.94	0.65
1:R:39:GLY:O	1:R:142:LEU:N	2.30	0.65
1:R:118:GLU:CB	1:R:138:TRP:HE3	2.08	0.65
1:R:122:THR:CA	1:R:136:ASP:HA	2.27	0.65
1:R:125:PHE:O	1:R:133:ARG:N	2.30	0.65
1:R:175:ALA:CB	1:R:224:GLU:O	2.43	0.65
1:R:111:PHE:O	1:R:111:PHE:CG	2.49	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:183:LEU:HD13	1:R:185:GLY:CA	2.27	0.65
1:R:192:VAL:HG13	1:R:192:VAL:O	1.96	0.65
1:R:36:GLN:HA	1:R:139:LEU:CB	2.26	0.65
1:R:168:SER:N	1:R:203:THR:O	2.29	0.64
1:R:38:PRO:HA	1:R:140:ARG:O	1.97	0.64
1:R:68:ARG:NH1	1:R:71:GLU:O	2.31	0.64
1:R:69:HIS:CA	1:R:70:GLY:O	2.46	0.64
1:R:30:VAL:O	1:R:51:LEU:HD11	1.97	0.64
1:R:114:ARG:HE	1:R:115:VAL:H	1.44	0.64
1:R:152:GLN:HB2	1:R:153:LYS:CD	2.27	0.64
1:R:220:THR:HA	1:R:235:THR:HG22	1.80	0.64
1:R:38:PRO:CD	1:R:140:ARG:HB2	2.28	0.64
1:R:91:ARG:HG2	1:R:92:LEU:N	2.13	0.64
1:R:186:MET:C	1:R:188:GLN:N	2.49	0.64
1:R:131:GLY:HA2	1:R:133:ARG:NH1	2.13	0.64
1:R:43:ASP:OD1	1:R:113:LEU:HA	1.97	0.64
1:R:47:LEU:HD12	1:R:108:LEU:O	1.97	0.64
1:R:86:TYR:CE1	1:R:94:PHE:CZ	2.86	0.64
1:R:161:VAL:HG23	1:R:161:VAL:O	1.98	0.64
1:R:172:ARG:HD3	1:R:173:PRO:N	2.13	0.64
1:R:215:ASP:C	1:R:238:LEU:HB2	2.19	0.64
1:R:61:VAL:H	1:R:127:THR:HA	1.63	0.64
1:R:181:SER:OG	1:R:184:GLY:HA2	1.98	0.63
1:R:173:PRO:O	1:R:225:HIS:CE1	2.51	0.63
1:R:186:MET:CE	1:R:207:ILE:HD12	2.29	0.63
1:R:63:GLN:HG2	1:R:81:THR:HG23	1.80	0.63
1:R:78:PHE:CD1	1:R:79:HIS:N	2.65	0.63
1:R:128:PHE:O	1:R:130:GLN:N	2.32	0.63
1:R:81:THR:O	1:R:98:ARG:NH2	2.31	0.63
1:R:37:VAL:H	1:R:139:LEU:CB	2.10	0.63
1:R:50:TYR:HB2	1:R:105:ASP:HB3	1.80	0.62
1:R:51:LEU:HD13	1:R:52:GLN:H	1.63	0.62
1:R:125:PHE:HD1	1:R:125:PHE:N	1.93	0.62
1:R:180:HIS:HD2	1:R:220:THR:CB	2.13	0.62
1:R:37:VAL:C	1:R:140:ARG:HB2	2.19	0.62
1:R:44:SER:CB	1:R:111:PHE:HA	2.29	0.62
1:R:44:SER:HB2	1:R:113:LEU:HD23	1.81	0.62
1:R:123:CYS:C	1:R:124:LEU:HD22	2.20	0.62
1:R:141:VAL:O	1:R:142:LEU:HD23	1.99	0.62
1:R:68:ARG:HH11	1:R:73:GLY:H	1.48	0.62
1:R:224:GLU:OE1	1:R:231:PRO:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:32:GLN:HG2	1:R:33:ALA:N	2.15	0.62
1:R:192:VAL:O	1:R:194:GLY:N	2.32	0.62
1:R:205:LEU:CA	1:R:206:TRP:CE2	2.83	0.62
1:R:217:LYS:HZ2	1:R:218:GLN:HE21	1.46	0.62
1:R:172:ARG:NH2	1:R:174:PRO:HD3	2.15	0.62
1:R:152:GLN:HB2	1:R:153:LYS:HD3	1.81	0.61
1:R:70:GLY:C	1:R:72:SER:H	2.03	0.61
1:R:173:PRO:HB2	1:R:225:HIS:CE1	2.36	0.61
1:R:90:LYS:HG2	1:R:91:ARG:N	2.14	0.61
1:R:154:VAL:HA	1:R:241:TYR:CE2	2.35	0.61
1:R:176:GLN:N	1:R:176:GLN:OE1	2.32	0.61
1:R:196:LEU:N	1:R:202:VAL:HG12	2.14	0.61
1:R:44:SER:OG	1:R:112:GLY:CA	2.47	0.61
1:R:102:GLU:HB2	1:R:103:LEU:C	2.21	0.61
1:R:38:PRO:HB3	1:R:140:ARG:HB3	1.81	0.61
1:R:95:VAL:O	1:R:96:ALA:HB3	2.01	0.61
1:R:124:LEU:HD13	1:R:134:SER:OG	2.00	0.61
1:R:155:GLN:NE2	1:R:211:SER:HA	2.16	0.61
1:R:176:GLN:OE1	1:R:224:GLU:HB3	2.00	0.61
1:R:33:ALA:HB1	1:R:48:PRO:O	1.99	0.61
1:R:95:VAL:O	1:R:96:ALA:CB	2.49	0.61
1:R:129:PRO:O	1:R:130:GLN:C	2.37	0.60
1:R:188:GLN:HB3	1:R:208:LEU:HD22	1.83	0.60
1:R:221:CYS:O	1:R:233:LEU:CA	2.49	0.60
1:R:215:ASP:HA	1:R:240:VAL:HG13	1.82	0.60
1:R:109:ARG:O	1:R:110:MET:CE	2.49	0.60
1:R:33:ALA:HB2	1:R:49:CYS:HA	1.83	0.60
1:R:117:ASP:HB2	1:R:141:VAL:CB	2.29	0.60
1:R:147:ASN:CG	1:R:168:SER:HA	2.21	0.60
1:R:190:SER:C	1:R:206:TRP:CZ3	2.74	0.60
1:R:49:CYS:HB3	1:R:66:TRP:CH2	2.36	0.60
1:R:78:PHE:HD2	1:R:108:LEU:HD21	1.66	0.60
1:R:147:ASN:OD1	1:R:168:SER:HA	2.02	0.60
1:R:161:VAL:O	1:R:163:MET:HB3	1.99	0.60
1:R:34:PRO:O	1:R:35:THR:OG1	2.21	0.59
1:R:68:ARG:NH1	1:R:73:GLY:H	1.99	0.59
1:R:162:PRO:HG3	1:R:209:VAL:HB	1.83	0.59
1:R:60:HIS:HB3	1:R:61:VAL:HA	1.84	0.59
1:R:159:GLU:H	1:R:160:PRO:HD3	1.66	0.59
1:R:104:ARG:H	1:R:104:ARG:CD	2.06	0.59
1:R:37:VAL:O	1:R:140:ARG:O	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:44:SER:HB3	1:R:111:PHE:CB	2.33	0.59
1:R:84:PRO:CB	1:R:94:PHE:CZ	2.86	0.59
1:R:237:SER:C	1:R:238:LEU:HD13	2.23	0.58
1:R:45:VAL:HG12	1:R:109:ARG:NH2	2.17	0.58
1:R:119:GLY:HA3	1:R:121:TYR:CE1	2.38	0.58
1:R:117:ASP:HB2	1:R:141:VAL:CG1	2.33	0.58
1:R:159:GLU:O	1:R:210:PRO:O	2.20	0.58
1:R:172:ARG:CZ	1:R:173:PRO:HA	2.32	0.58
1:R:181:SER:CB	1:R:219:VAL:HG23	2.17	0.58
1:R:46:THR:CB	1:R:109:ARG:HA	2.27	0.58
1:R:61:VAL:HB	1:R:63:GLN:HE22	1.69	0.58
1:R:63:GLN:H	1:R:126:VAL:HG23	1.69	0.58
1:R:118:GLU:HG2	1:R:141:VAL:HG11	1.86	0.58
1:R:124:LEU:C	1:R:125:PHE:CD1	2.70	0.58
1:R:127:THR:HB	1:R:129:PRO:HD2	1.85	0.58
1:R:157:THR:OG1	1:R:211:SER:HB3	2.04	0.58
1:R:37:VAL:O	1:R:37:VAL:HG13	2.03	0.58
1:R:143:ALA:O	1:R:173:PRO:CD	2.52	0.58
1:R:175:ALA:HB1	1:R:224:GLU:O	2.04	0.58
1:R:44:SER:O	1:R:45:VAL:HG13	2.04	0.57
1:R:91:ARG:O	1:R:92:LEU:HB2	2.03	0.57
1:R:104:ARG:H	1:R:104:ARG:HH11	1.50	0.57
1:R:151:VAL:HG22	1:R:152:GLN:N	2.19	0.57
1:R:152:GLN:HB2	1:R:153:LYS:CG	2.34	0.57
1:R:128:PHE:N	1:R:129:PRO:CD	2.67	0.57
1:R:136:ASP:CG	1:R:137:ILE:N	2.58	0.57
1:R:38:PRO:CB	1:R:140:ARG:HB2	2.35	0.57
1:R:91:ARG:NH1	1:R:92:LEU:HD22	2.20	0.57
1:R:227:SER:O	1:R:228:PHE:C	2.43	0.57
1:R:43:ASP:H	1:R:44:SER:HB2	1.70	0.56
1:R:93:GLU:CG	1:R:111:PHE:CZ	2.87	0.56
1:R:144:LYS:CE	1:R:145:PRO:O	2.38	0.56
1:R:215:ASP:OD1	1:R:215:ASP:N	2.37	0.56
1:R:205:LEU:C	1:R:206:TRP:CD1	2.79	0.56
1:R:30:VAL:C	1:R:51:LEU:HD11	2.26	0.56
1:R:49:CYS:O	1:R:106:ALA:O	2.23	0.56
1:R:61:VAL:HG23	1:R:63:GLN:OE1	2.05	0.56
1:R:145:PRO:HB3	1:R:171:GLY:CA	2.36	0.56
1:R:92:LEU:HD12	1:R:111:PHE:O	2.04	0.56
1:R:38:PRO:HB3	1:R:140:ARG:CB	2.35	0.56
1:R:217:LYS:HD2	1:R:217:LYS:C	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:103:LEU:HD13	1:R:103:LEU:N	2.21	0.56
1:R:84:PRO:HB3	1:R:94:PHE:CZ	2.41	0.56
1:R:102:GLU:OE1	1:R:104:ARG:HA	2.06	0.56
1:R:192:VAL:O	1:R:203:THR:OG1	2.17	0.56
1:R:59:THR:CB	1:R:129:PRO:CG	2.84	0.56
1:R:162:PRO:HD2	1:R:209:VAL:HG23	1.88	0.56
1:R:221:CYS:O	1:R:233:LEU:HA	2.06	0.56
1:R:38:PRO:HA	1:R:140:ARG:C	2.27	0.55
1:R:47:LEU:CD1	1:R:108:LEU:HB2	2.36	0.55
1:R:122:THR:HB	1:R:136:ASP:CB	2.33	0.55
1:R:35:THR:O	1:R:36:GLN:NE2	2.38	0.55
1:R:162:PRO:CG	1:R:209:VAL:HB	2.36	0.55
1:R:180:HIS:HD2	1:R:220:THR:HB	1.71	0.55
1:R:36:GLN:C	1:R:139:LEU:HB3	2.26	0.55
1:R:92:LEU:HG	1:R:110:MET:SD	2.47	0.55
1:R:199:THR:C	1:R:200:VAL:HG22	2.27	0.55
1:R:218:GLN:HG2	1:R:219:VAL:N	2.22	0.55
1:R:186:MET:HE1	1:R:207:ILE:HD12	1.87	0.55
1:R:60:HIS:HB3	1:R:61:VAL:HG13	1.89	0.55
1:R:64:LEU:CD1	1:R:106:ALA:HB3	2.35	0.55
1:R:70:GLY:O	1:R:72:SER:N	2.33	0.55
1:R:129:PRO:O	1:R:131:GLY:N	2.39	0.55
1:R:131:GLY:HA2	1:R:133:ARG:HH11	1.72	0.55
1:R:147:ASN:ND2	1:R:168:SER:HA	2.22	0.55
1:R:194:GLY:O	1:R:195:PHE:HB3	2.07	0.55
1:R:110:MET:CE	1:R:110:MET:HA	2.35	0.55
1:R:180:HIS:CD2	1:R:220:THR:HB	2.42	0.55
1:R:222:LYS:HA	1:R:233:LEU:CB	2.26	0.55
1:R:36:GLN:O	1:R:140:ARG:HG3	2.07	0.55
1:R:151:VAL:HG22	1:R:152:GLN:H	1.70	0.55
1:R:189:THR:CG2	1:R:207:ILE:HG22	2.36	0.55
1:R:205:LEU:N	1:R:206:TRP:NE1	2.55	0.54
1:R:212:SER:OG	1:R:213:GLN:N	2.40	0.54
1:R:32:GLN:H	1:R:51:LEU:HD22	1.72	0.54
1:R:93:GLU:HG3	1:R:111:PHE:HZ	1.68	0.54
1:R:194:GLY:O	1:R:195:PHE:CB	2.54	0.54
1:R:66:TRP:CE2	1:R:108:LEU:HD23	2.42	0.54
1:R:147:ASN:OD1	1:R:169:THR:N	2.39	0.54
1:R:142:LEU:CB	1:R:172:ARG:HG3	2.36	0.54
1:R:213:GLN:NE2	1:R:240:VAL:HG12	2.22	0.54
1:R:33:ALA:C	1:R:35:THR:HG23	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:61:VAL:HB	1:R:63:GLN:NE2	2.23	0.54
1:R:118:GLU:HG3	1:R:138:TRP:HE3	1.73	0.54
1:R:46:THR:OG1	1:R:47:LEU:N	2.38	0.54
1:R:161:VAL:H	1:R:208:LEU:CA	2.19	0.54
1:R:201:THR:O	1:R:202:VAL:HG12	2.08	0.54
1:R:31:VAL:CG2	1:R:133:ARG:HH21	2.15	0.54
1:R:78:PHE:CD2	1:R:108:LEU:HD21	2.43	0.54
1:R:45:VAL:O	1:R:110:MET:CA	2.55	0.54
1:R:48:PRO:HA	1:R:107:SER:CB	2.38	0.54
1:R:179:TRP:HA	1:R:220:THR:O	2.08	0.54
1:R:64:LEU:HD12	1:R:66:TRP:HE1	1.73	0.54
1:R:78:PHE:HE1	1:R:80:GLN:HB2	1.72	0.54
1:R:148:THR:O	1:R:149:ALA:HB2	2.08	0.54
1:R:109:ARG:O	1:R:110:MET:HE1	2.07	0.53
1:R:217:LYS:O	1:R:237:SER:HA	2.08	0.53
1:R:238:LEU:N	1:R:238:LEU:HD22	2.24	0.53
1:R:87:SER:O	1:R:89:SER:N	2.41	0.53
1:R:189:THR:HA	1:R:208:LEU:CD1	2.34	0.53
1:R:63:GLN:H	1:R:126:VAL:CG2	2.21	0.53
1:R:84:PRO:HB2	1:R:94:PHE:CZ	2.43	0.53
1:R:103:LEU:HB3	1:R:104:ARG:HH12	1.73	0.53
1:R:82:GLN:HA	1:R:82:GLN:NE2	2.22	0.53
1:R:118:GLU:CB	1:R:138:TRP:HB2	2.33	0.53
1:R:171:GLY:O	1:R:201:THR:CG2	2.46	0.53
1:R:128:PHE:N	1:R:129:PRO:HD2	2.24	0.53
1:R:133:ARG:O	1:R:134:SER:HB3	2.09	0.53
1:R:162:PRO:HD3	1:R:209:VAL:O	2.09	0.53
1:R:65:THR:HG22	1:R:124:LEU:HD23	1.90	0.52
1:R:41:LEU:N	1:R:143:ALA:HB2	2.21	0.52
1:R:185:GLY:O	1:R:186:MET:HG3	2.08	0.52
1:R:132:SER:O	1:R:133:ARG:CB	2.51	0.52
1:R:172:ARG:HD3	1:R:173:PRO:CG	2.38	0.52
1:R:183:LEU:CD1	1:R:185:GLY:HA3	2.40	0.52
1:R:162:PRO:HD2	1:R:163:MET:HA	1.90	0.52
1:R:73:GLY:N	1:R:74:SER:HA	2.22	0.52
1:R:143:ALA:O	1:R:173:PRO:HD2	2.09	0.52
1:R:216:GLY:H	1:R:238:LEU:CA	2.23	0.52
1:R:218:GLN:HA	1:R:236:VAL:O	2.08	0.52
1:R:155:GLN:CD	1:R:211:SER:CA	2.67	0.52
1:R:162:PRO:N	1:R:163:MET:HB3	2.22	0.52
1:R:205:LEU:HA	1:R:206:TRP:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:138:TRP:O	1:R:139:LEU:CD2	2.42	0.52
1:R:144:LYS:HE3	1:R:145:PRO:CD	2.34	0.52
1:R:197:SER:C	1:R:199:THR:H	2.13	0.52
1:R:91:ARG:HH11	1:R:92:LEU:HD13	1.74	0.52
1:R:167:VAL:HA	1:R:204:SER:HA	1.90	0.52
1:R:66:TRP:CZ2	1:R:108:LEU:HD23	2.44	0.51
1:R:175:ALA:O	1:R:176:GLN:HB3	2.09	0.51
1:R:186:MET:SD	1:R:207:ILE:CB	2.94	0.51
1:R:50:TYR:HB2	1:R:105:ASP:CB	2.40	0.51
1:R:44:SER:HB3	1:R:111:PHE:HA	1.89	0.51
1:R:117:ASP:HB3	1:R:141:VAL:HB	1.93	0.51
1:R:206:TRP:N	1:R:206:TRP:CE3	2.78	0.51
1:R:55:ASN:N	1:R:57:GLU:H	2.07	0.51
1:R:103:LEU:HB3	1:R:104:ARG:NH1	2.25	0.51
1:R:114:ARG:HE	1:R:115:VAL:N	2.07	0.51
1:R:212:SER:O	1:R:213:GLN:OE1	2.29	0.51
1:R:109:ARG:HD3	1:R:109:ARG:C	2.31	0.51
1:R:51:LEU:HD13	1:R:52:GLN:N	2.26	0.51
1:R:98:ARG:HG2	1:R:100:GLY:H	1.75	0.51
1:R:35:THR:HB	1:R:137:ILE:HG21	1.93	0.51
1:R:44:SER:OG	1:R:113:LEU:HB3	2.11	0.51
1:R:63:GLN:HB3	1:R:81:THR:OG1	2.12	0.50
1:R:167:VAL:HG13	1:R:169:THR:OG1	2.11	0.50
1:R:55:ASN:H	1:R:57:GLU:N	2.08	0.50
1:R:93:GLU:CG	1:R:111:PHE:HZ	2.22	0.50
1:R:114:ARG:NE	1:R:115:VAL:N	2.59	0.50
1:R:165:ARG:HB3	1:R:165:ARG:HH11	1.76	0.50
1:R:173:PRO:HB3	1:R:226:GLU:OE1	2.11	0.50
1:R:189:THR:CB	1:R:207:ILE:HG22	2.41	0.50
1:R:195:PHE:C	1:R:196:LEU:HD13	2.29	0.50
1:R:208:LEU:CD1	1:R:208:LEU:N	2.75	0.50
1:R:62:SER:N	1:R:126:VAL:O	2.42	0.50
1:R:161:VAL:N	1:R:208:LEU:HA	2.22	0.50
1:R:215:ASP:CB	1:R:240:VAL:HG22	2.30	0.50
1:R:90:LYS:H	1:R:90:LYS:NZ	2.04	0.50
1:R:118:GLU:CG	1:R:138:TRP:HE3	2.24	0.50
1:R:141:VAL:O	1:R:142:LEU:CD2	2.59	0.50
1:R:190:SER:O	1:R:205:LEU:CG	2.57	0.50
1:R:112:GLY:CA	1:R:113:LEU:HG	2.41	0.50
1:R:192:VAL:HG12	1:R:204:SER:N	2.26	0.50
1:R:60:HIS:CE1	1:R:104:ARG:NH2	2.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:114:ARG:NE	1:R:115:VAL:H	2.09	0.50
1:R:114:ARG:HD3	1:R:116:GLU:OE2	2.12	0.50
1:R:218:GLN:CG	1:R:219:VAL:N	2.74	0.50
1:R:80:GLN:NE2	1:R:98:ARG:H	2.10	0.49
1:R:172:ARG:HD3	1:R:173:PRO:HG3	1.94	0.49
1:R:175:ALA:HB2	1:R:224:GLU:O	2.11	0.49
1:R:139:LEU:O	1:R:141:VAL:CG1	2.60	0.49
1:R:177:ILE:CG2	1:R:223:VAL:HG22	2.42	0.49
1:R:121:TYR:N	1:R:137:ILE:O	2.44	0.49
1:R:75:MET:HE2	1:R:75:MET:H	1.76	0.49
1:R:141:VAL:O	1:R:142:LEU:HG	2.13	0.49
1:R:69:HIS:HB2	1:R:72:SER:OG	2.13	0.49
1:R:112:GLY:HA3	1:R:113:LEU:CG	2.43	0.49
1:R:215:ASP:CB	1:R:216:GLY:CA	2.67	0.49
1:R:38:PRO:CD	1:R:140:ARG:HD2	2.37	0.49
1:R:127:THR:O	1:R:130:GLN:O	2.31	0.49
1:R:218:GLN:HG2	1:R:219:VAL:H	1.78	0.49
1:R:82:GLN:HA	1:R:98:ARG:NH1	2.27	0.49
1:R:119:GLY:HA3	1:R:121:TYR:CZ	2.48	0.49
1:R:240:VAL:O	1:R:241:TYR:HD2	1.94	0.49
1:R:55:ASN:HB3	1:R:56:MET:SD	2.53	0.49
1:R:60:HIS:HB3	1:R:61:VAL:CA	2.43	0.49
1:R:65:THR:C	1:R:66:TRP:CD1	2.86	0.49
1:R:118:GLU:HA	1:R:119:GLY:HA3	1.49	0.49
1:R:41:LEU:HD21	1:R:114:ARG:CA	2.43	0.49
1:R:112:GLY:HA3	1:R:113:LEU:CB	2.42	0.49
1:R:172:ARG:HD3	1:R:173:PRO:HD3	1.95	0.49
1:R:196:LEU:HD13	1:R:196:LEU:H	1.73	0.49
1:R:137:ILE:C	1:R:138:TRP:CD1	2.86	0.48
1:R:165:ARG:HB3	1:R:165:ARG:NH1	2.28	0.48
1:R:118:GLU:HB3	1:R:138:TRP:CB	2.32	0.48
1:R:139:LEU:O	1:R:141:VAL:HG13	2.13	0.48
1:R:41:LEU:CD1	1:R:113:LEU:O	2.60	0.48
1:R:58:VAL:HG23	1:R:103:LEU:HD21	1.95	0.48
1:R:74:SER:O	1:R:75:MET:HB3	2.14	0.48
1:R:80:GLN:HG3	1:R:83:GLY:O	2.13	0.48
1:R:161:VAL:CA	1:R:163:MET:HB3	2.43	0.48
1:R:194:GLY:HA2	1:R:203:THR:HA	1.94	0.48
1:R:225:HIS:HD2	1:R:227:SER:HB2	1.77	0.48
1:R:119:GLY:O	1:R:120:SER:C	2.49	0.48
1:R:205:LEU:C	1:R:206:TRP:CD2	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:75:MET:HG2	1:R:75:MET:O	2.13	0.48
1:R:90:LYS:HG2	1:R:91:ARG:H	1.78	0.48
1:R:120:SER:CA	1:R:138:TRP:CD1	2.82	0.48
1:R:143:ALA:O	1:R:172:ARG:CB	2.58	0.48
1:R:162:PRO:N	1:R:163:MET:CA	2.77	0.48
1:R:188:GLN:HB3	1:R:208:LEU:CD2	2.43	0.48
1:R:192:VAL:HG11	1:R:204:SER:H	1.76	0.47
1:R:33:ALA:HB1	1:R:49:CYS:HA	1.95	0.47
1:R:157:THR:HA	1:R:211:SER:OG	2.14	0.47
1:R:51:LEU:H	1:R:105:ASP:CG	2.16	0.47
1:R:201:THR:CG2	1:R:202:VAL:H	2.03	0.47
1:R:92:LEU:HB3	1:R:110:MET:SD	2.55	0.47
1:R:47:LEU:HD12	1:R:47:LEU:H	1.80	0.47
1:R:65:THR:O	1:R:123:CYS:HA	2.14	0.47
1:R:78:PHE:CD1	1:R:78:PHE:C	2.88	0.47
1:R:172:ARG:CZ	1:R:174:PRO:HD3	2.45	0.47
1:R:173:PRO:O	1:R:225:HIS:ND1	2.48	0.47
1:R:199:THR:O	1:R:199:THR:CG2	2.62	0.47
1:R:224:GLU:O	1:R:225:HIS:CB	2.57	0.47
1:R:233:LEU:N	1:R:233:LEU:HD23	2.29	0.47
1:R:109:ARG:O	1:R:110:MET:HE2	2.14	0.47
1:R:198:GLY:O	1:R:199:THR:CB	2.63	0.47
1:R:38:PRO:CB	1:R:140:ARG:CB	2.93	0.46
1:R:102:GLU:H	1:R:103:LEU:HA	1.81	0.46
1:R:118:GLU:OE1	1:R:138:TRP:HB2	2.14	0.46
1:R:192:VAL:CG1	1:R:192:VAL:O	2.63	0.46
1:R:68:ARG:HD2	1:R:68:ARG:N	2.29	0.46
1:R:70:GLY:C	1:R:72:SER:N	2.67	0.46
1:R:47:LEU:CD1	1:R:108:LEU:O	2.64	0.46
1:R:183:LEU:C	1:R:185:GLY:N	2.69	0.46
1:R:241:TYR:HA	1:R:242:TYR:C	2.36	0.46
1:R:47:LEU:HD12	1:R:47:LEU:N	2.30	0.46
1:R:162:PRO:CD	1:R:163:MET:HA	2.46	0.46
1:R:186:MET:SD	1:R:207:ILE:CD1	3.00	0.46
1:R:63:GLN:C	1:R:79:HIS:CE1	2.89	0.46
1:R:114:ARG:NH2	1:R:115:VAL:O	2.49	0.46
1:R:141:VAL:O	1:R:142:LEU:CG	2.63	0.46
1:R:161:VAL:HA	1:R:207:ILE:O	2.16	0.46
1:R:87:SER:C	1:R:89:SER:N	2.66	0.46
1:R:137:ILE:HG23	1:R:138:TRP:N	2.30	0.46
1:R:230:LYS:HA	1:R:231:PRO:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:75:MET:HE2	1:R:75:MET:N	2.31	0.46
1:R:112:GLY:HA3	1:R:113:LEU:HG	1.96	0.46
1:R:145:PRO:HB2	1:R:146:GLN:H	1.40	0.46
1:R:183:LEU:C	1:R:185:GLY:H	2.18	0.46
1:R:41:LEU:C	1:R:43:ASP:HA	2.36	0.46
1:R:78:PHE:CD2	1:R:108:LEU:HD11	2.50	0.46
1:R:120:SER:CA	1:R:138:TRP:CG	2.89	0.46
1:R:198:GLY:O	1:R:199:THR:HB	2.16	0.46
1:R:35:THR:O	1:R:35:THR:OG1	2.34	0.46
1:R:38:PRO:HA	1:R:39:GLY:HA3	1.60	0.46
1:R:159:GLU:C	1:R:210:PRO:HA	2.36	0.46
1:R:128:PHE:H	1:R:129:PRO:HD2	1.80	0.45
1:R:35:THR:O	1:R:139:LEU:HD23	2.16	0.45
1:R:135:VAL:CG1	1:R:136:ASP:O	2.63	0.45
1:R:155:GLN:OE1	1:R:210:PRO:O	2.34	0.45
1:R:177:ILE:CG2	1:R:223:VAL:HA	2.46	0.45
1:R:47:LEU:HD11	1:R:108:LEU:CB	2.45	0.45
1:R:153:LYS:O	1:R:239:THR:HB	2.17	0.45
1:R:177:ILE:HG21	1:R:223:VAL:HG22	1.99	0.45
1:R:190:SER:O	1:R:206:TRP:CZ3	2.69	0.45
1:R:41:LEU:HD21	1:R:114:ARG:N	2.32	0.45
1:R:61:VAL:CG2	1:R:63:GLN:OE1	2.64	0.45
1:R:179:TRP:CG	1:R:207:ILE:CG2	3.00	0.45
1:R:221:CYS:O	1:R:234:LEU:N	2.49	0.45
1:R:45:VAL:O	1:R:110:MET:HB3	2.16	0.45
1:R:195:PHE:N	1:R:196:LEU:HD13	2.32	0.45
1:R:179:TRP:CG	1:R:207:ILE:HG23	2.51	0.45
1:R:45:VAL:O	1:R:110:MET:C	2.55	0.45
1:R:68:ARG:HH12	1:R:73:GLY:C	2.19	0.45
1:R:90:LYS:HB3	1:R:90:LYS:HZ2	1.82	0.45
1:R:66:TRP:CD1	1:R:66:TRP:N	2.83	0.45
1:R:91:ARG:HH12	1:R:92:LEU:HD22	1.81	0.45
1:R:216:GLY:N	1:R:238:LEU:HB2	2.32	0.45
1:R:61:VAL:HG23	1:R:126:VAL:O	2.17	0.45
1:R:128:PHE:H	1:R:129:PRO:CD	2.30	0.45
1:R:180:HIS:CD2	1:R:220:THR:CB	2.97	0.45
1:R:145:PRO:CD	1:R:171:GLY:HA3	2.47	0.44
1:R:127:THR:OG1	1:R:131:GLY:O	2.30	0.44
1:R:172:ARG:O	1:R:174:PRO:HD3	2.17	0.44
1:R:44:SER:HB3	1:R:111:PHE:CA	2.47	0.44
1:R:68:ARG:HG2	1:R:72:SER:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:156:LEU:HD12	1:R:157:THR:N	2.33	0.44
1:R:193:PRO:O	1:R:195:PHE:N	2.50	0.44
1:R:92:LEU:N	1:R:92:LEU:CD1	2.80	0.44
1:R:147:ASN:HB3	1:R:167:VAL:O	2.18	0.44
1:R:181:SER:OG	1:R:186:MET:CE	2.64	0.44
1:R:217:LYS:NZ	1:R:218:GLN:NE2	2.63	0.44
1:R:181:SER:HA	1:R:219:VAL:HA	1.99	0.44
1:R:182:ASP:O	1:R:183:LEU:C	2.55	0.44
1:R:32:GLN:HG2	1:R:33:ALA:H	1.82	0.44
1:R:90:LYS:NZ	1:R:90:LYS:HB3	2.33	0.44
1:R:62:SER:HB2	1:R:104:ARG:HG2	1.99	0.44
1:R:190:SER:HB2	1:R:206:TRP:HZ3	1.82	0.44
1:R:152:GLN:HG3	1:R:163:MET:SD	2.57	0.44
1:R:184:GLY:O	1:R:186:MET:N	2.51	0.44
1:R:203:THR:O	1:R:203:THR:HG23	2.17	0.44
1:R:222:LYS:HE2	1:R:231:PRO:CB	2.45	0.44
1:R:214:VAL:O	1:R:215:ASP:C	2.56	0.44
1:R:92:LEU:HD11	1:R:112:GLY:H	1.83	0.43
1:R:177:ILE:HG22	1:R:222:LYS:C	2.38	0.43
1:R:195:PHE:H	1:R:196:LEU:HD13	1.82	0.43
1:R:206:TRP:O	1:R:206:TRP:CE3	2.61	0.43
1:R:219:VAL:HG22	1:R:220:THR:N	2.33	0.43
1:R:55:ASN:O	1:R:55:ASN:ND2	2.47	0.43
1:R:91:ARG:HD2	1:R:92:LEU:HD13	2.00	0.43
1:R:117:ASP:O	1:R:121:TYR:HE1	2.00	0.43
1:R:145:PRO:N	1:R:171:GLY:HA2	2.32	0.43
1:R:61:VAL:N	1:R:127:THR:HG22	2.34	0.43
1:R:68:ARG:O	1:R:69:HIS:HB3	2.18	0.43
1:R:118:GLU:HB3	1:R:120:SER:H	1.82	0.43
1:R:186:MET:CE	1:R:209:VAL:HG22	2.47	0.43
1:R:50:TYR:HB2	1:R:105:ASP:CG	2.38	0.43
1:R:145:PRO:CB	1:R:171:GLY:CA	2.96	0.43
1:R:190:SER:C	1:R:206:TRP:CH2	2.91	0.43
1:R:61:VAL:HB	1:R:63:GLN:OE1	2.19	0.43
1:R:68:ARG:CB	1:R:70:GLY:HA3	2.46	0.43
1:R:168:SER:O	1:R:202:VAL:C	2.57	0.43
1:R:172:ARG:CB	1:R:173:PRO:CD	2.87	0.43
1:R:233:LEU:O	1:R:234:LEU:HD23	2.19	0.43
1:R:65:THR:CA	1:R:78:PHE:O	2.52	0.43
1:R:136:ASP:OD1	1:R:136:ASP:C	2.57	0.43
1:R:169:THR:HA	1:R:202:VAL:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:45:VAL:O	1:R:110:MET:CB	2.67	0.43
1:R:68:ARG:O	1:R:69:HIS:CB	2.66	0.43
1:R:188:GLN:O	1:R:189:THR:HG22	2.18	0.43
1:R:41:LEU:HD22	1:R:43:ASP:CG	2.39	0.43
1:R:103:LEU:O	1:R:104:ARG:O	2.37	0.43
1:R:142:LEU:HB3	1:R:143:ALA:H	1.74	0.43
1:R:162:PRO:N	1:R:163:MET:HA	2.34	0.43
1:R:55:ASN:C	1:R:56:MET:SD	2.97	0.42
1:R:204:SER:HB2	1:R:206:TRP:NE1	2.11	0.42
1:R:225:HIS:CD2	1:R:227:SER:HB2	2.53	0.42
1:R:31:VAL:HA	1:R:51:LEU:CD2	2.33	0.42
1:R:79:HIS:CE1	1:R:81:THR:OG1	2.72	0.42
1:R:41:LEU:HD22	1:R:41:LEU:HA	1.74	0.42
1:R:41:LEU:HD21	1:R:114:ARG:HA	2.01	0.42
1:R:68:ARG:HG3	1:R:71:GLU:N	2.34	0.42
1:R:116:GLU:O	1:R:117:ASP:OD1	2.37	0.42
1:R:218:GLN:N	1:R:238:LEU:HD21	2.34	0.42
1:R:78:PHE:CZ	1:R:80:GLN:HB2	2.54	0.42
1:R:91:ARG:NH1	1:R:92:LEU:HD13	2.34	0.42
1:R:143:ALA:O	1:R:173:PRO:HD3	2.19	0.42
1:R:168:SER:HB3	1:R:203:THR:HG23	2.02	0.42
1:R:68:ARG:NH1	1:R:73:GLY:C	2.73	0.42
1:R:176:GLN:C	1:R:177:ILE:HD13	2.40	0.42
1:R:186:MET:HB3	1:R:188:GLN:HB2	2.02	0.42
1:R:159:GLU:OE2	1:R:160:PRO:CG	2.64	0.42
1:R:161:VAL:HA	1:R:208:LEU:HA	2.01	0.42
1:R:35:THR:O	1:R:139:LEU:CD2	2.68	0.42
1:R:180:HIS:HD2	1:R:220:THR:OG1	2.03	0.42
1:R:51:LEU:HD22	1:R:51:LEU:HA	1.83	0.41
1:R:60:HIS:HB3	1:R:61:VAL:HG12	2.00	0.41
1:R:152:GLN:HG3	1:R:163:MET:CG	2.50	0.41
1:R:228:PHE:HD2	1:R:230:LYS:O	2.03	0.41
1:R:41:LEU:HD13	1:R:43:ASP:OD2	2.21	0.41
1:R:36:GLN:NE2	1:R:139:LEU:HD21	2.35	0.41
1:R:124:LEU:HD22	1:R:124:LEU:N	2.36	0.41
1:R:144:LYS:HE3	1:R:144:LYS:HB2	1.87	0.41
1:R:91:ARG:HH11	1:R:92:LEU:CD1	2.33	0.41
1:R:142:LEU:HB3	1:R:172:ARG:CG	2.43	0.41
1:R:152:GLN:CB	1:R:153:LYS:HG2	2.48	0.41
1:R:39:GLY:HA3	1:R:140:ARG:O	2.20	0.41
1:R:216:GLY:N	1:R:238:LEU:H	2.11	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:211:SER:O	1:R:212:SER:HB3	2.21	0.41
1:R:122:THR:CB	1:R:136:ASP:CA	2.59	0.41
1:R:150:GLU:N	1:R:165:ARG:O	2.51	0.41
1:R:168:SER:OG	1:R:203:THR:HG22	2.21	0.41
1:R:184:GLY:HA2	1:R:186:MET:HE3	2.03	0.41
1:R:159:GLU:CD	1:R:159:GLU:N	2.74	0.40
1:R:64:LEU:HD11	1:R:106:ALA:CB	2.48	0.40
1:R:38:PRO:CA	1:R:140:ARG:CB	2.95	0.40
1:R:39:GLY:O	1:R:142:LEU:O	2.40	0.40
1:R:43:ASP:H	1:R:113:LEU:HB3	1.86	0.40
1:R:149:ALA:CA	1:R:165:ARG:O	2.62	0.40
1:R:155:GLN:H	1:R:241:TYR:CB	2.35	0.40
1:R:217:LYS:HZ3	1:R:218:GLN:HE21	1.69	0.40
1:R:43:ASP:N	1:R:113:LEU:HB3	2.36	0.40
1:R:94:PHE:CD1	1:R:94:PHE:N	2.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	R	211/221 (96%)	111 (53%)	50 (24%)	50 (24%)	0 1

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	45	VAL
1	R	55	ASN
1	R	72	SER
1	R	96	ALA
1	R	98	ARG
1	R	104	ARG

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Mol	Chain	Res	Type
1	R	117	ASP
1	R	130	GLN
1	R	133	ARG
1	R	134	SER
1	R	137	ILE
1	R	145	PRO
1	R	194	GLY
1	R	197	SER
1	R	199	THR
1	R	201	THR
1	R	215	ASP
1	R	229	GLU
1	R	240	VAL
1	R	81	THR
1	R	87	SER
1	R	88	GLU
1	R	146	GLN
1	R	195	PHE
1	R	210	PRO
1	R	212	SER
1	R	237	SER
1	R	54	PRO
1	R	71	GLU
1	R	92	LEU
1	R	93	GLU
1	R	105	ASP
1	R	159	GLU
1	R	163	MET
1	R	176	GLN
1	R	185	GLY
1	R	193	PRO
1	R	231	PRO
1	R	34	PRO
1	R	70	GLY
1	R	75	MET
1	R	138	TRP
1	R	149	ALA
1	R	152	GLN
1	R	129	PRO
1	R	196	LEU
1	R	58	VAL
1	R	33	ALA

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Mol	Chain	Res	Type
1	R	172	ARG
1	R	202	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	R	185/193 (96%)	116 (63%)	69 (37%)	0 1

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	41	LEU
1	R	43	ASP
1	R	44	SER
1	R	47	LEU
1	R	49	CYS
1	R	51	LEU
1	R	55	ASN
1	R	56	MET
1	R	62	SER
1	R	64	LEU
1	R	65	THR
1	R	68	ARG
1	R	75	MET
1	R	78	PHE
1	R	82	GLN
1	R	90	LYS
1	R	91	ARG
1	R	93	GLU
1	R	94	PHE
1	R	103	LEU
1	R	104	ARG
1	R	109	ARG
1	R	110	MET
1	R	113	LEU

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Mol	Chain	Res	Type
1	R	114	ARG
1	R	122	THR
1	R	125	PHE
1	R	126	VAL
1	R	128	PHE
1	R	132	SER
1	R	133	ARG
1	R	135	VAL
1	R	136	ASP
1	R	137	ILE
1	R	146	GLN
1	R	148	THR
1	R	150	GLU
1	R	154	VAL
1	R	159	GLU
1	R	165	ARG
1	R	168	SER
1	R	169	THR
1	R	172	ARG
1	R	177	ILE
1	R	178	THR
1	R	180	HIS
1	R	182	ASP
1	R	183	LEU
1	R	186	MET
1	R	189	THR
1	R	191	GLN
1	R	196	LEU
1	R	200	VAL
1	R	204	SER
1	R	205	LEU
1	R	206	TRP
1	R	208	LEU
1	R	209	VAL
1	R	215	ASP
1	R	218	GLN
1	R	229	GLU
1	R	230	LYS
1	R	232	GLN
1	R	233	LEU
1	R	236	VAL
1	R	238	LEU

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Mol	Chain	Res	Type
1	R	239	THR
1	R	240	VAL
1	R	241	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	36	GLN
1	R	52	GLN
1	R	60	HIS
1	R	79	HIS
1	R	80	GLN
1	R	155	GLN
1	R	180	HIS
1	R	218	GLN
1	R	225	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	R	213/221 (96%)	-0.36	0	100	100	62, 98, 133, 166	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.