Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:41 pm BST

PDB ID	:	5EW5
Title	:	Crystal Structure of Colicin E9 In Complex with Its Immunity Protein Im9
Authors	:	Klein, A.; Wojdyla, J.A.; Kleanthous, C.
Deposited on	:	2015-11-20
Resolution	:	3.20 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 following versions of software and data (see references ①) were used in the production of this report:

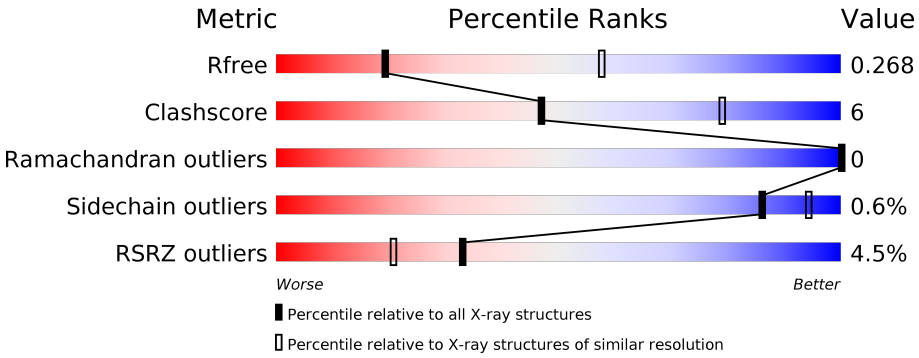
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 on 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	A	582	% 72% 12% 16%
1	B	582	% 72% 12% 16%
1	C	582	5% 71% 13% 16%
1	D	582	3% 70% 14% 16%
2	E	94	% 86% • 12%
2	F	94	3% 80% 9% 12%

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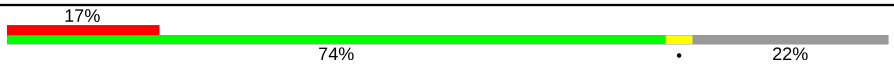
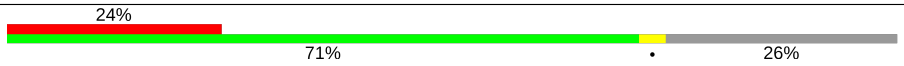
Mol	Chain	Length	Quality of chain
2	G	94	
2	H	94	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17397 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 Colicin-E9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3737	2300	687	740	10			
1	B	490	Total	C	N	O	S	0	0	0
			3737	2300	687	740	10			
1	C	490	Total	C	N	O	S	0	1	0
			3748	2306	691	741	10			
1	D	490	Total	C	N	O	S	0	0	0
			3737	2300	687	740	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	324	CYS	TYR	engineered mutation	UNP P09883
A	447	CYS	LEU	engineered mutation	UNP P09883
A	448	ALA	ASP	engineered mutation	UNP P09883
A	449	MET	LYS	engineered mutation	UNP P09883
B	324	CYS	TYR	engineered mutation	UNP P09883
B	447	CYS	LEU	engineered mutation	UNP P09883
B	448	ALA	ASP	engineered mutation	UNP P09883
B	449	MET	LYS	engineered mutation	UNP P09883
C	324	CYS	TYR	engineered mutation	UNP P09883
C	447	CYS	LEU	engineered mutation	UNP P09883
C	448	ALA	ASP	engineered mutation	UNP P09883
C	449	MET	LYS	engineered mutation	UNP P09883
D	324	CYS	TYR	engineered mutation	UNP P09883
D	447	CYS	LEU	engineered mutation	UNP P09883
D	448	ALA	ASP	engineered mutation	UNP P09883
D	449	MET	LYS	engineered mutation	UNP P09883

- Molecule 2 is a protein called Colicin-E9 immunity protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	83	Total	C	N	O	S	0	0	0
			651	406	105	138	2			
2	F	83	Total	C	N	O	S	0	0	0
			651	406	105	138	2			
2	G	73	Total	C	N	O	S	0	0	0
			569	353	89	125	2			
2	H	70	Total	C	N	O	S	0	0	0
			545	340	84	119	2			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	87	LEU	-	expression tag	UNP P13479
E	88	GLU	-	expression tag	UNP P13479
E	89	HIS	-	expression tag	UNP P13479
E	90	HIS	-	expression tag	UNP P13479
E	91	HIS	-	expression tag	UNP P13479
E	92	HIS	-	expression tag	UNP P13479
E	93	HIS	-	expression tag	UNP P13479
E	94	HIS	-	expression tag	UNP P13479
F	87	LEU	-	expression tag	UNP P13479
F	88	GLU	-	expression tag	UNP P13479
F	89	HIS	-	expression tag	UNP P13479
F	90	HIS	-	expression tag	UNP P13479
F	91	HIS	-	expression tag	UNP P13479
F	92	HIS	-	expression tag	UNP P13479
F	93	HIS	-	expression tag	UNP P13479
F	94	HIS	-	expression tag	UNP P13479
G	87	LEU	-	expression tag	UNP P13479
G	88	GLU	-	expression tag	UNP P13479
G	89	HIS	-	expression tag	UNP P13479
G	90	HIS	-	expression tag	UNP P13479
G	91	HIS	-	expression tag	UNP P13479
G	92	HIS	-	expression tag	UNP P13479
G	93	HIS	-	expression tag	UNP P13479
G	94	HIS	-	expression tag	UNP P13479
H	87	LEU	-	expression tag	UNP P13479
H	88	GLU	-	expression tag	UNP P13479
H	89	HIS	-	expression tag	UNP P13479
H	90	HIS	-	expression tag	UNP P13479
H	91	HIS	-	expression tag	UNP P13479
H	92	HIS	-	expression tag	UNP P13479
H	93	HIS	-	expression tag	UNP P13479
H	94	HIS	-	expression tag	UNP P13479

- Molecule 3 is water.

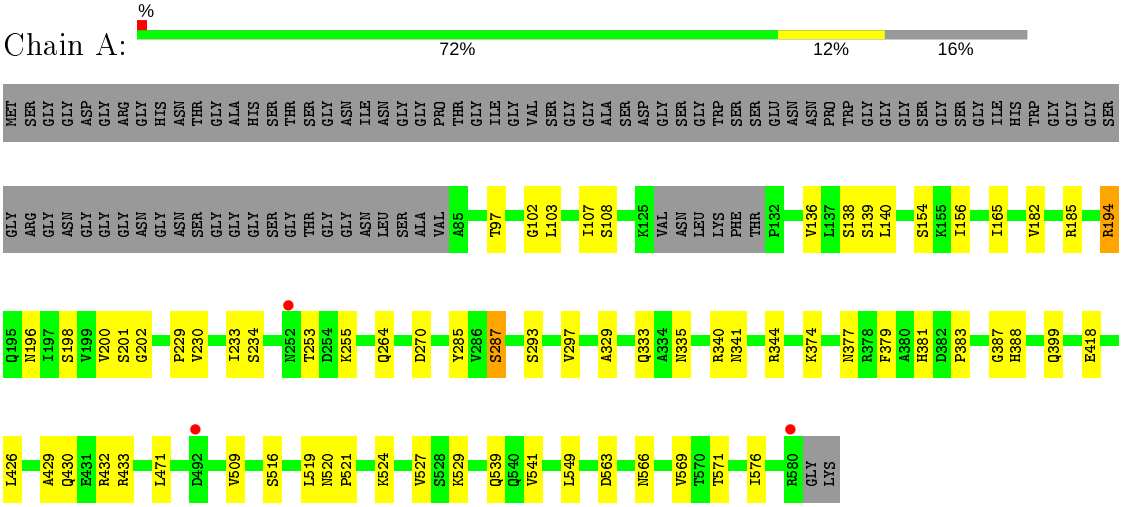
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	6	Total O 6 6	0	0
3	B	3	Total O 3 3	0	0
3	C	5	Total O 5 5	0	0
3	D	5	Total O 5 5	0	0
3	E	1	Total O 1 1	0	0
3	F	1	Total O 1 1	0	0
3	G	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

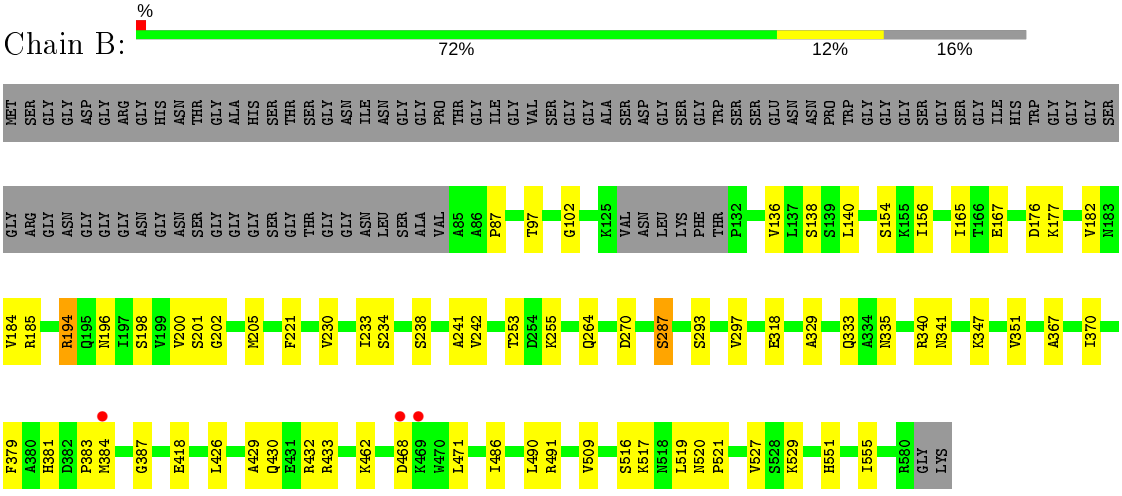
- Molecule 1: Colicin-E9

Chain A:



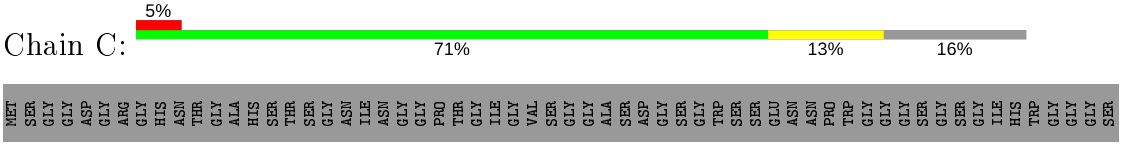
- Molecule 1: Colicin-E9

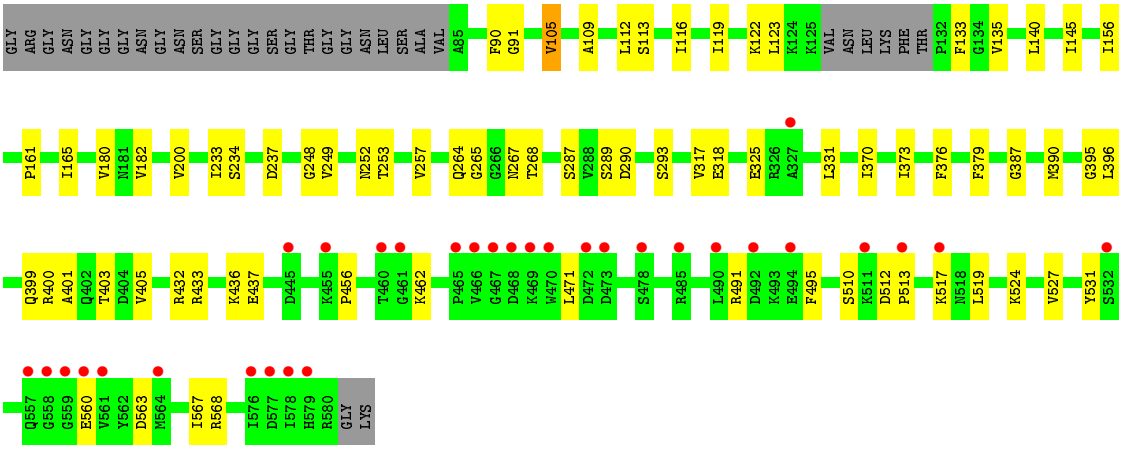
Chain B:



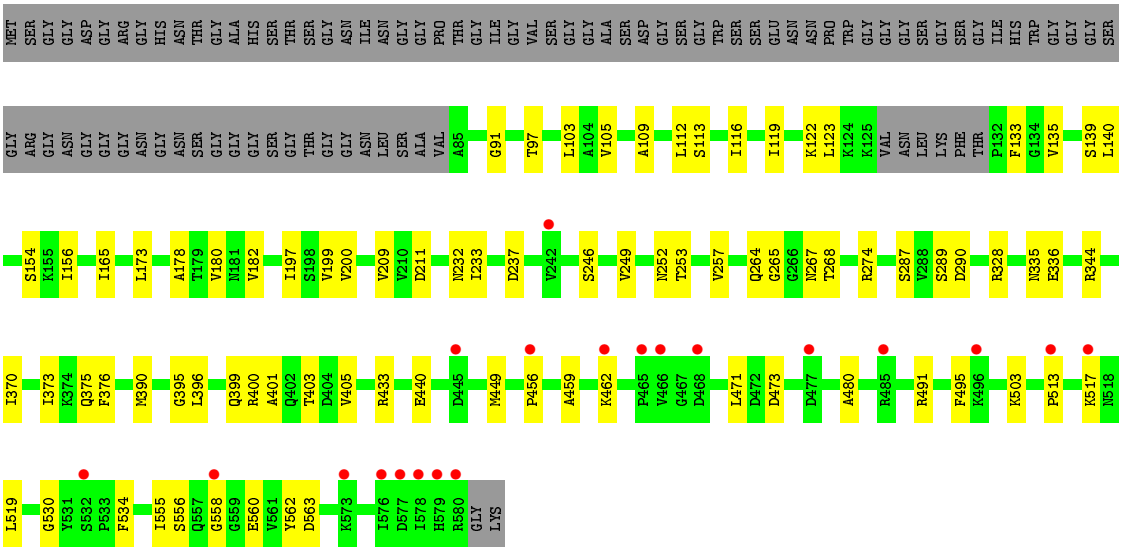
- Molecule 1: Colicin-E9

Chain C:

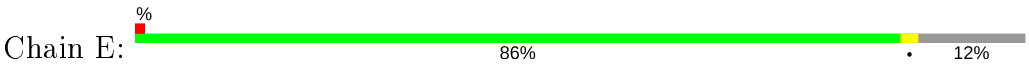


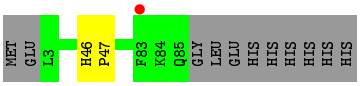


• Molecule 1: Colicin-E9

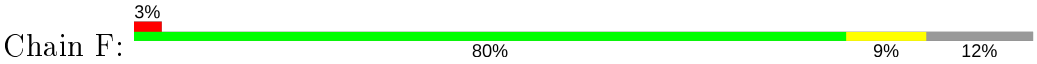


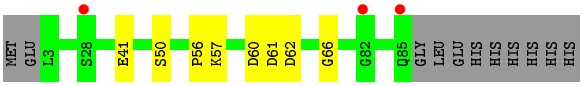
• Molecule 2: Colicin-E9 immunity protein



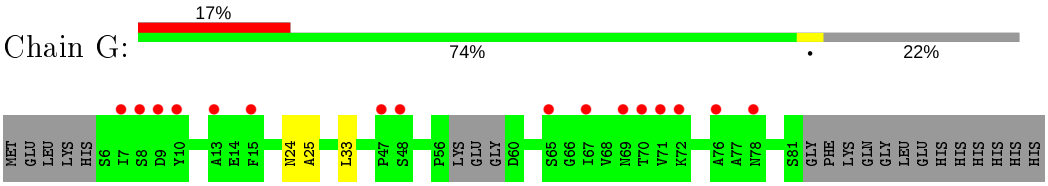


• Molecule 2: Colicin-E9 immunity protein

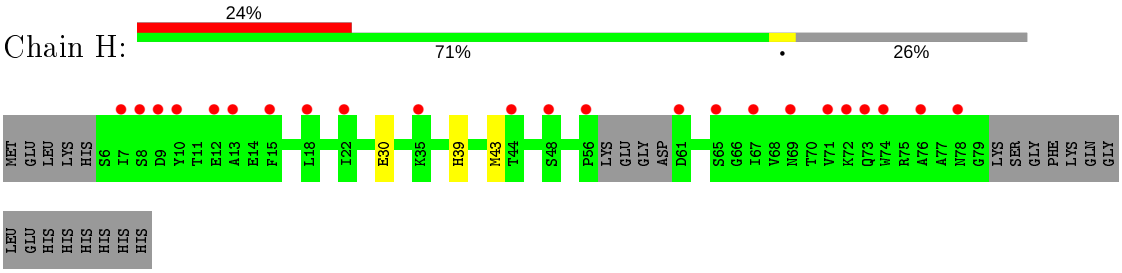




• Molecule 2: Colicin-E9 immunity protein



- Molecule 2: Colicin-E9 immunity protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.89Å 116.05Å 150.37Å 90.00° 93.72° 90.00°	Depositor
Resolution (Å)	29.60 – 3.20 29.61 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.60-3.20) 98.9 (29.61-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.01	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.212 , 0.271 0.211 , 0.268	Depositor DCC
R_{free} test set	2705 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	68.9	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 48.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17397	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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	A	0.49	0/3801	0.70	1/5139 (0.0%)
1	B	0.49	0/3801	0.71	1/5139 (0.0%)
1	C	0.48	0/3812	0.68	1/5153 (0.0%)
1	D	0.49	0/3801	0.69	0/5139
2	E	0.46	0/664	0.60	0/899
2	F	0.45	0/664	0.58	0/899
2	G	0.43	0/579	0.53	0/787
2	H	0.43	0/555	0.52	0/755
All	All	0.48	0/17677	0.68	3/23910 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	194	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	B	194	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C	180	VAL	CB-CA-C	-5.35	101.24	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	A	3737	0	3711	50	0
1	B	3737	0	3711	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3748	0	3723	50	0
1	D	3737	0	3711	66	0
2	E	651	0	614	1	0
2	F	651	0	614	5	0
2	G	569	0	527	2	0
2	H	545	0	504	2	0
3	A	6	0	0	0	0
3	B	3	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
All	All	17397	0	17115	212	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 6.

All (212) 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:D:103:LEU:O	1:D:232:ASN:OD1	1.96	0.82
1:A:138:SER:O	1:A:196:ASN:HB2	1.87	0.74
1:A:329:ALA:O	1:A:333:GLN:HG3	1.89	0.71
1:A:340:ARG:HD2	1:D:396:LEU:HD13	1.74	0.70
1:C:265:GLY:HA2	1:C:268:THR:HG22	1.73	0.69
1:C:264:GLN:HG3	1:C:264:GLN:O	1.93	0.67
1:D:264:GLN:HG3	1:D:264:GLN:O	1.93	0.67
1:B:341:ASN:HB3	1:B:426:LEU:HD12	1.75	0.67
1:D:109:ALA:HB3	1:D:237:ASP:HB3	1.77	0.65
1:D:265:GLY:HA2	1:D:268:THR:HG22	1.79	0.64
1:D:268:THR:OG1	1:D:289:SER:HB3	1.98	0.64
1:B:138:SER:O	1:B:196:ASN:HB2	1.98	0.63
1:C:165:ILE:HG22	1:C:182:VAL:HB	1.78	0.63
1:D:370:ILE:O	1:D:373:ILE:HG22	1.99	0.63
1:A:140:LEU:HD21	1:A:156:ILE:HD12	1.79	0.63
1:D:471:LEU:HD11	1:D:519:LEU:HD11	1.81	0.63
1:B:340:ARG:HD2	1:C:396:LEU:HD13	1.80	0.61
1:D:165:ILE:HG22	1:D:182:VAL:HB	1.80	0.61
1:A:381:HIS:O	1:A:383:PRO:HD3	2.00	0.61
1:C:105:VAL:O	1:C:233:ILE:HA	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ILE:CG2	1:A:182:VAL:HB	2.31	0.60
1:A:335:ASN:OD1	1:A:433:ARG:HD2	2.01	0.60
1:A:509:VAL:O	1:A:516:SER:HB2	2.02	0.60
1:B:379:PHE:CG	1:B:387:GLY:HA3	2.37	0.60
1:C:513:PRO:O	1:C:517:LYS:HB2	2.02	0.59
1:C:456:PRO:HA	1:C:495:PHE:O	2.02	0.59
1:C:471:LEU:HD11	1:C:519:LEU:HD11	1.83	0.59
1:A:270:ASP:HB3	1:A:287:SER:HB2	1.84	0.59
1:C:109:ALA:HB3	1:C:237:ASP:HB3	1.84	0.58
1:A:293:SER:O	1:A:297:VAL:HG23	2.03	0.58
1:B:381:HIS:O	1:B:383:PRO:HD3	2.04	0.58
1:A:136:VAL:HA	1:A:198:SER:HB3	1.85	0.58
1:C:265:GLY:CA	1:C:268:THR:HG22	2.34	0.57
1:B:140:LEU:HD21	1:B:156:ILE:HD12	1.87	0.57
1:C:401:ALA:O	1:C:405:VAL:HG23	2.04	0.57
1:D:105:VAL:O	1:D:233:ILE:HA	2.06	0.56
1:D:373:ILE:HD12	1:D:395:GLY:CA	2.34	0.56
1:D:200:VAL:HG11	1:D:264:GLN:OE1	2.06	0.56
1:D:119:ILE:O	1:D:123:LEU:HB2	2.06	0.56
1:A:341:ASN:HB3	1:A:426:LEU:HD12	1.89	0.55
1:B:329:ALA:O	1:B:333:GLN:HG3	2.07	0.54
1:D:119:ILE:HD12	1:D:135:VAL:HG11	1.87	0.54
1:B:136:VAL:HA	1:B:198:SER:HB3	1.89	0.54
2:F:41:GLU:OE2	2:F:50:SER:HB3	2.08	0.54
1:A:524:LYS:HA	1:A:527:VAL:HG22	1.89	0.54
1:D:449:MET:CE	1:D:558:GLY:H	2.20	0.53
1:A:341:ASN:HB3	1:A:426:LEU:CD1	2.39	0.53
1:B:264:GLN:O	1:B:264:GLN:HG3	2.09	0.53
1:A:102:GLY:HA3	1:A:230:VAL:O	2.09	0.53
1:B:418:GLU:CG	1:C:403:THR:HG23	2.39	0.53
1:C:373:ILE:HD12	1:C:395:GLY:CA	2.39	0.53
1:B:270:ASP:HB3	1:B:287:SER:HB2	1.90	0.52
1:A:418:GLU:CG	1:D:403:THR:HG23	2.39	0.52
1:D:449:MET:HE1	1:D:558:GLY:H	1.75	0.52
1:D:335:ASN:OD1	1:D:433:ARG:NE	2.41	0.52
1:D:328:ARG:HA	1:D:440:GLU:HG3	1.92	0.52
1:C:200:VAL:HG11	1:C:264:GLN:OE1	2.10	0.52
1:D:376:PHE:CE2	1:D:390:MET:HB3	2.45	0.52
2:H:39:HIS:O	2:H:43:MET:HG2	2.09	0.52
1:A:340:ARG:HD2	1:D:396:LEU:CD1	2.40	0.52
1:C:119:ILE:HD12	1:C:135:VAL:HG11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ASN:HB3	1:B:426:LEU:CD1	2.41	0.51
1:C:165:ILE:CG2	1:C:182:VAL:HB	2.41	0.51
1:C:267:ASN:HB3	1:C:290:ASP:HB2	1.92	0.51
1:D:373:ILE:HD12	1:D:395:GLY:HA2	1.93	0.51
1:D:165:ILE:CG2	1:D:182:VAL:HB	2.41	0.51
1:B:233:ILE:HG22	1:B:234:SER:N	2.25	0.51
1:C:531:TYR:HB3	2:H:30:GLU:OE1	2.10	0.51
1:C:370:ILE:O	1:C:373:ILE:HG22	2.10	0.50
1:D:249:VAL:O	1:D:249:VAL:HG13	2.12	0.50
1:B:293:SER:O	1:B:297:VAL:HG23	2.12	0.50
1:C:123:LEU:HD12	1:C:133:PHE:HE1	1.77	0.50
1:D:513:PRO:O	1:D:517:LYS:HB2	2.10	0.50
1:D:401:ALA:O	1:D:405:VAL:HG23	2.12	0.50
1:C:91:GLY:CA	1:C:116:ILE:HD12	2.40	0.50
1:D:449:MET:CE	1:D:558:GLY:N	2.75	0.49
1:D:560:GLU:HB2	1:D:563:ASP:HB3	1.95	0.49
1:A:233:ILE:HG22	1:A:234:SER:N	2.27	0.49
1:A:549:LEU:CD2	1:A:569:VAL:HG22	2.43	0.49
1:C:122:LYS:HE3	1:C:257:VAL:HG23	1.95	0.49
1:D:140:LEU:HD11	1:D:197:ILE:HD13	1.94	0.49
1:D:97:THR:HG22	1:D:154:SER:OG	2.12	0.49
1:C:140:LEU:HD21	1:C:156:ILE:HD12	1.93	0.49
1:B:165:ILE:CG2	1:B:182:VAL:HB	2.43	0.49
1:D:473:ASP:HB2	1:D:480:ALA:HB2	1.95	0.48
1:A:379:PHE:CG	1:A:387:GLY:HA3	2.48	0.48
1:C:249:VAL:HG13	1:C:249:VAL:O	2.14	0.48
1:B:194:ARG:HH11	1:B:194:ARG:HG2	1.78	0.48
1:C:567:ILE:O	1:C:568:ARG:NH1	2.47	0.48
1:D:123:LEU:HD12	1:D:133:PHE:HE1	1.78	0.48
1:D:140:LEU:HD21	1:D:156:ILE:HD12	1.96	0.48
1:C:91:GLY:HA3	1:C:116:ILE:HD12	1.97	0.47
1:A:97:THR:HG22	1:A:154:SER:OG	2.14	0.47
1:D:376:PHE:HE2	1:D:390:MET:HB3	1.79	0.47
1:B:264:GLN:O	1:B:264:GLN:CG	2.63	0.47
1:B:509:VAL:O	1:B:516:SER:HB2	2.14	0.47
1:C:252:ASN:OD1	1:C:253:THR:N	2.47	0.47
1:C:268:THR:OG1	1:C:289:SER:HB3	2.14	0.47
1:C:462:LYS:HA	1:C:491:ARG:HH21	1.80	0.47
1:B:102:GLY:HA3	1:B:230:VAL:O	2.14	0.47
1:D:560:GLU:HB3	1:D:563:ASP:HB2	1.95	0.47
1:D:456:PRO:HA	1:D:495:PHE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:SER:C	1:A:140:LEU:HD12	2.36	0.46
1:B:426:LEU:O	1:B:430:GLN:N	2.43	0.46
1:B:184:VAL:HA	1:B:205:MET:HE1	1.98	0.46
1:C:265:GLY:HA2	1:C:268:THR:CG2	2.43	0.46
2:F:56:PRO:HG2	2:F:62:ASP:HB3	1.98	0.46
1:D:560:GLU:CB	1:D:563:ASP:HB2	2.46	0.46
1:A:107:ILE:HD12	1:A:108:SER:O	2.16	0.46
1:B:462:LYS:HA	1:B:491:ARG:NH2	2.31	0.46
1:B:471:LEU:HD11	1:B:519:LEU:CD1	2.46	0.46
1:B:97:THR:HG22	1:B:154:SER:OG	2.16	0.46
1:D:335:ASN:O	1:D:336:GLU:C	2.53	0.46
1:A:194:ARG:HG2	1:A:194:ARG:HH11	1.80	0.45
1:A:529:LYS:HG3	1:A:529:LYS:O	2.16	0.45
1:C:433:ARG:O	1:C:437:GLU:N	2.49	0.45
1:D:112:LEU:O	1:D:113:SER:C	2.54	0.45
1:B:185:ARG:HH21	1:B:270:ASP:CG	2.20	0.45
1:D:105:VAL:HG13	1:D:233:ILE:HG12	1.97	0.45
1:A:520:ASN:HB3	1:A:521:PRO:HD2	1.99	0.45
1:B:384:MET:HE1	1:C:325:GLU:C	2.36	0.45
1:C:524:LYS:HA	1:C:527:VAL:HG22	1.99	0.45
1:B:201:SER:OG	1:B:202:GLY:N	2.49	0.45
1:A:140:LEU:HD21	1:A:156:ILE:CD1	2.47	0.45
1:B:367:ALA:HA	1:B:370:ILE:HG22	1.99	0.45
1:D:265:GLY:CA	1:D:268:THR:HG22	2.45	0.45
1:D:376:PHE:CD1	1:D:376:PHE:N	2.83	0.45
1:A:344:ARG:NH2	1:A:418:GLU:OE2	2.47	0.45
1:D:91:GLY:CA	1:D:116:ILE:HD12	2.46	0.44
1:A:140:LEU:N	1:A:140:LEU:HD12	2.32	0.44
1:D:267:ASN:HB3	1:D:290:ASP:HB2	1.98	0.44
1:B:551:HIS:CE1	1:B:555:ILE:HD11	2.53	0.44
1:C:119:ILE:O	1:C:123:LEU:HB2	2.17	0.44
1:D:178:ALA:C	1:D:209:VAL:HG12	2.38	0.44
1:C:379:PHE:CG	1:C:387:GLY:HA3	2.53	0.44
1:D:449:MET:O	1:D:555:ILE:HG22	2.18	0.44
1:C:432:ARG:O	1:C:436:LYS:HB2	2.18	0.44
2:F:61:ASP:OD2	2:F:66:GLY:HA3	2.17	0.44
1:B:347:LYS:O	1:B:351:VAL:HG23	2.18	0.44
2:F:56:PRO:CG	2:F:62:ASP:HB3	2.47	0.43
1:A:374:LYS:O	1:A:377:ASN:HB2	2.19	0.43
1:A:429:ALA:HA	1:A:432:ARG:NH1	2.33	0.43
1:D:534:PHE:CE1	2:G:33:LEU:HD12	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:PHE:N	1:D:376:PHE:HD1	2.16	0.43
1:A:335:ASN:OD1	1:A:433:ARG:CD	2.65	0.43
1:A:471:LEU:HD11	1:A:519:LEU:HD11	2.00	0.43
1:B:529:LYS:O	1:B:529:LYS:HG3	2.19	0.43
1:C:90:PHE:CG	1:C:161:PRO:HD3	2.54	0.43
1:D:252:ASN:OD1	1:D:253:THR:N	2.52	0.43
2:G:24:ASN:O	2:G:25:ALA:HB3	2.19	0.43
1:A:201:SER:OG	1:A:202:GLY:N	2.51	0.43
1:D:459:ALA:HA	1:D:562:TYR:HB3	2.00	0.43
1:D:399:GLN:CG	1:D:400:ARG:N	2.80	0.43
1:D:462:LYS:HA	1:D:491:ARG:HH21	1.84	0.43
1:A:165:ILE:CD1	1:A:285:TYR:CG	3.02	0.43
1:A:519:LEU:HD21	1:A:527:VAL:HG11	2.01	0.43
1:B:520:ASN:HB3	1:B:521:PRO:HD2	2.00	0.43
1:C:373:ILE:HD12	1:C:395:GLY:HA2	2.01	0.42
1:D:139:SER:C	1:D:140:LEU:HD12	2.38	0.42
1:D:503:LYS:HG3	1:D:530:GLY:HA3	2.00	0.42
1:C:145:ILE:HG13	1:C:248:GLY:HA3	2.01	0.42
1:D:122:LYS:HE3	1:D:257:VAL:HG23	2.00	0.42
1:C:399:GLN:CG	1:C:400:ARG:N	2.83	0.42
1:A:471:LEU:HD11	1:A:519:LEU:CD1	2.50	0.42
1:A:418:GLU:HG3	1:D:403:THR:HG23	2.01	0.42
1:B:176:ASP:OD1	1:B:177:LYS:N	2.53	0.42
1:B:221:PHE:CD1	1:B:221:PHE:N	2.88	0.42
1:D:173:LEU:HD22	1:D:180:VAL:HG22	2.02	0.42
1:A:103:LEU:HG	1:A:229:PRO:HG2	2.02	0.41
1:A:264:GLN:HG3	1:A:264:GLN:O	2.20	0.41
1:A:426:LEU:O	1:A:430:GLN:N	2.44	0.41
1:B:167:GLU:OE1	1:B:167:GLU:N	2.45	0.41
1:A:185:ARG:HH21	1:A:270:ASP:CG	2.22	0.41
1:B:335:ASN:OD1	1:B:433:ARG:HD2	2.19	0.41
1:A:399:GLN:CD	1:D:344:ARG:HD2	2.40	0.41
1:D:375:GLN:C	1:D:376:PHE:HD1	2.24	0.41
1:C:112:LEU:O	1:C:113:SER:C	2.58	0.41
2:F:57:LYS:HB2	2:F:60:ASP:OD2	2.20	0.41
1:A:200:VAL:HG12	1:A:201:SER:N	2.35	0.41
1:A:388:HIS:CG	1:A:388:HIS:O	2.74	0.41
1:A:539:GLN:HB3	1:A:571:THR:HB	2.02	0.41
1:B:462:LYS:HA	1:B:491:ARG:HH21	1.84	0.41
1:D:91:GLY:HA3	1:D:116:ILE:HD12	2.02	0.41
1:C:560:GLU:HB2	1:C:563:ASP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:LEU:CD2	1:D:199:VAL:HG12	2.51	0.41
2:E:46:HIS:HA	2:E:47:PRO:HD3	1.95	0.41
1:B:87:PRO:HG2	1:B:241:ALA:HA	2.03	0.41
1:B:253:THR:O	1:B:255:LYS:HG2	2.21	0.41
1:B:200:VAL:HG12	1:B:201:SER:N	2.35	0.41
1:C:331:LEU:HD13	1:C:437:GLU:HA	2.03	0.41
1:A:563:ASP:O	1:A:566:ASN:HB3	2.20	0.41
1:A:541:VAL:HG21	1:A:576:ILE:HD12	2.03	0.41
1:B:270:ASP:HB3	1:B:287:SER:CB	2.50	0.41
1:B:468:ASP:OD1	1:B:517:LYS:HG2	2.21	0.41
1:B:429:ALA:HA	1:B:432:ARG:NH1	2.36	0.41
1:C:376:PHE:CE2	1:C:390:MET:HB3	2.56	0.41
1:A:140:LEU:CD1	1:A:140:LEU:N	2.84	0.41
1:D:211:ASP:OD1	1:D:274:ARG:HD2	2.21	0.41
1:C:233:ILE:HG22	1:C:234:SER:N	2.36	0.40
1:B:233:ILE:CG2	1:B:234:SER:N	2.85	0.40
1:D:449:MET:HE3	1:D:558:GLY:N	2.35	0.40
1:D:560:GLU:CB	1:D:563:ASP:CB	2.99	0.40
1:A:253:THR:O	1:A:255:LYS:HG2	2.21	0.40
1:C:90:PHE:CE2	1:C:161:PRO:HG3	2.55	0.40
1:B:486:ILE:HG22	1:B:490:LEU:HD12	2.03	0.40
1:B:519:LEU:HD21	1:B:527:VAL:HG11	2.02	0.40
1:C:376:PHE:N	1:C:376:PHE:CD1	2.88	0.40
1:C:90:PHE:CE2	1:C:109:ALA:HA	2.56	0.40
1:C:317:VAL:HG23	1:C:318:GLU:N	2.37	0.40
1:C:510:SER:HB3	1:C:527:VAL:HG23	2.03	0.40
1:D:268:THR:HA	1:D:289:SER:HA	2.03	0.40
1:D:449:MET:HE1	1:D:556:SER:C	2.42	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	A	486/582 (84%)	445 (92%)	41 (8%)	0	100	100
1	B	486/582 (84%)	446 (92%)	40 (8%)	0	100	100
1	C	487/582 (84%)	460 (94%)	27 (6%)	0	100	100
1	D	486/582 (84%)	457 (94%)	29 (6%)	0	100	100
2	E	81/94 (86%)	78 (96%)	3 (4%)	0	100	100
2	F	81/94 (86%)	76 (94%)	5 (6%)	0	100	100
2	G	69/94 (73%)	66 (96%)	3 (4%)	0	100	100
2	H	66/94 (70%)	64 (97%)	2 (3%)	0	100	100
All	All	2242/2704 (83%)	2092 (93%)	150 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	A	405/459 (88%)	404 (100%)	1 (0%)	93	98
1	B	405/459 (88%)	401 (99%)	4 (1%)	76	90
1	C	406/459 (88%)	402 (99%)	4 (1%)	76	90
1	D	405/459 (88%)	403 (100%)	2 (0%)	88	95
2	E	74/84 (88%)	74 (100%)	0	100	100
2	F	74/84 (88%)	74 (100%)	0	100	100
2	G	66/84 (79%)	66 (100%)	0	100	100
2	H	62/84 (74%)	62 (100%)	0	100	100
All	All	1897/2172 (87%)	1886 (99%)	11 (1%)	86	94

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	287	SER
1	B	238	SER

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Mol	Chain	Res	Type
1	B	242	VAL
1	B	287	SER
1	B	318	GLU
1	C	105	VAL
1	C	287	SER
1	C	293	SER
1	C	512	ASP
1	D	246	SER
1	D	287	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	232	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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	A	490/582 (84%)	-0.20	3 (0%) 89 83	36, 76, 115, 151	0
1	B	490/582 (84%)	-0.27	3 (0%) 89 83	34, 75, 132, 194	0
1	C	490/582 (84%)	0.09	32 (6%) 18 11	30, 82, 185, 229	0
1	D	490/582 (84%)	-0.01	20 (4%) 37 24	35, 78, 178, 226	0
2	E	83/94 (88%)	-0.02	1 (1%) 79 67	63, 92, 113, 122	0
2	F	83/94 (88%)	0.11	3 (3%) 42 27	63, 97, 127, 138	0
2	G	73/94 (77%)	1.22	16 (21%) 0 0	112, 163, 203, 250	0
2	H	70/94 (74%)	1.47	23 (32%) 0 0	108, 171, 199, 228	0
All	All	2269/2704 (83%)	0.00	101 (4%) 33 21	30, 82, 178, 250	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	7	ILE	6.4
2	G	8	SER	5.6
1	D	558	GLY	5.3
1	C	466	VAL	5.1
2	H	7	ILE	4.8
2	H	15	PHE	4.5
2	G	9	ASP	4.3
1	C	578	ILE	4.3
1	C	513	PRO	4.2
2	H	78	ASN	4.0
2	H	10	TYR	3.9
1	D	517	LYS	3.9
1	C	467	GLY	3.9
2	G	15	PHE	3.8
2	H	65	SER	3.8
2	G	10	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	485	ARG	3.8
1	D	466	VAL	3.7
2	H	8	SER	3.6
1	C	468	ASP	3.6
1	C	470	TRP	3.6
2	G	69	ASN	3.5
1	C	558	GLY	3.5
1	C	465	PRO	3.5
1	D	513	PRO	3.5
1	D	462	LYS	3.5
2	G	78	ASN	3.4
2	H	76	ALA	3.4
2	H	9	ASP	3.3
2	H	18	LEU	3.3
1	C	517	LYS	3.2
2	G	65	SER	3.2
1	C	557	GLN	3.1
1	A	492	ASP	3.0
1	D	579	HIS	3.0
2	H	48	SER	3.0
1	D	465	PRO	3.0
2	G	47	PRO	3.0
1	D	577	ASP	2.9
1	C	579	HIS	2.9
1	C	511	LYS	2.9
1	D	580	ARG	2.9
2	G	76	ALA	2.9
2	H	69	ASN	2.9
2	G	13	ALA	2.8
1	C	485	ARG	2.8
1	C	561	VAL	2.8
2	E	83	PHE	2.7
1	D	578	ILE	2.7
1	C	460	THR	2.7
1	C	473	ASP	2.7
1	D	468	ASP	2.7
1	B	469	LYS	2.7
2	F	85	GLN	2.6
1	D	477	ASP	2.6
1	C	559	GLY	2.6
1	C	455	LYS	2.5
1	C	492	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	576	ILE	2.5
1	D	242	VAL	2.5
1	C	560	GLU	2.5
1	C	564	MET	2.4
2	G	72	LYS	2.4
2	H	61	ASP	2.4
1	C	532	SER	2.4
2	F	28	SER	2.4
2	G	67	ILE	2.4
2	H	22	ILE	2.4
2	H	72	LYS	2.3
2	H	44	THR	2.3
2	H	35	LYS	2.3
2	H	73	GLN	2.3
2	F	82	GLY	2.3
2	H	12	GLU	2.3
1	C	490	LEU	2.3
2	G	48	SER	2.3
1	D	573	LYS	2.3
2	H	74	TRP	2.3
1	C	577	ASP	2.3
1	D	532	SER	2.2
1	B	468	ASP	2.2
1	D	456	PRO	2.2
1	C	445	ASP	2.2
1	D	496	LYS	2.2
1	C	469	LYS	2.2
1	A	580	ARG	2.2
1	D	445	ASP	2.2
1	C	327	ALA	2.2
1	C	494	GLU	2.1
1	B	384	MET	2.1
1	D	576	ILE	2.1
2	G	71	VAL	2.1
1	C	461	GLY	2.1
2	H	13	ALA	2.1
1	C	478	SER	2.1
2	G	70	THR	2.0
2	H	71	VAL	2.0
1	C	472	ASP	2.0
1	A	252	ASN	2.0
2	H	67	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	56	PRO	2.0

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 carbohydrates 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.