Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 03:18 PM EDT

PDB ID	:	6QHD
Title	:	Lysine acetylated and tyrosine phosphorylated STAT3 in a complex with DNA
Authors	:	Arbely, E.; Belo, Y.; Shahar, A.; Zarivach, R.
Deposited on	:	2019-01-16
Resolution	:	2.85 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 (i) 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 (1)) were used in the production of this report:

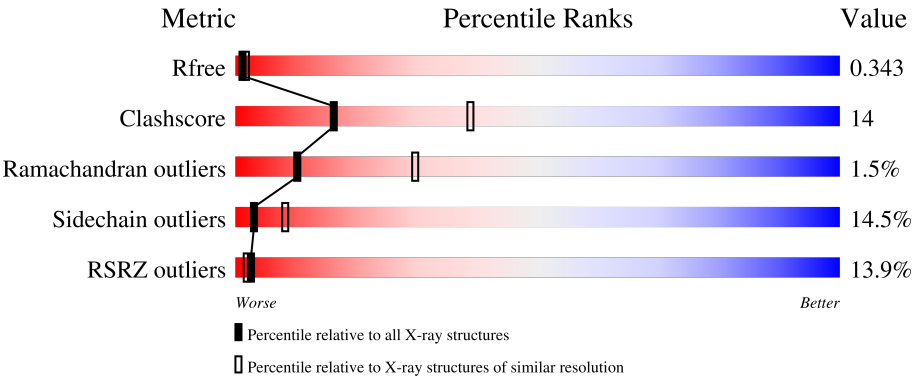
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	A	596	13% 58% 26% 5% • 11%
1	B	596	13% 59% 24% 6% • 11%
2	C	18	72% 17% 11%
3	D	18	67% 22% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9454 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 Signal transducer and activator of transcription 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	530	Total	C	N	O	P	S	0	1	0
			4310	2756	728	796	1	29			
1	B	532	Total	C	N	O	P	S	0	0	0
			4323	2767	731	797	1	27			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	631	SER	LYS	conflict	UNP P40763
B	631	SER	LYS	conflict	UNP P40763

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*AP*GP*AP*TP*TP*TP*AP*CP*GP*GP*GP*AP*AP*AP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	18	Total	C	N	O	P	0	0	0
			372	178	74	103	17			

- Molecule 3 is a DNA chain called DNA (5'-D(*TP*GP*CP*AP*TP*TP*TP*CP*CP*CP*GP*TP*AP*AP*AP*TP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	18	Total	C	N	O	P	0	0	0
			360	175	59	109	17			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		
4	B	36	Total	O	0	0
			36	36		

Continued on next page...

Continued from previous page...

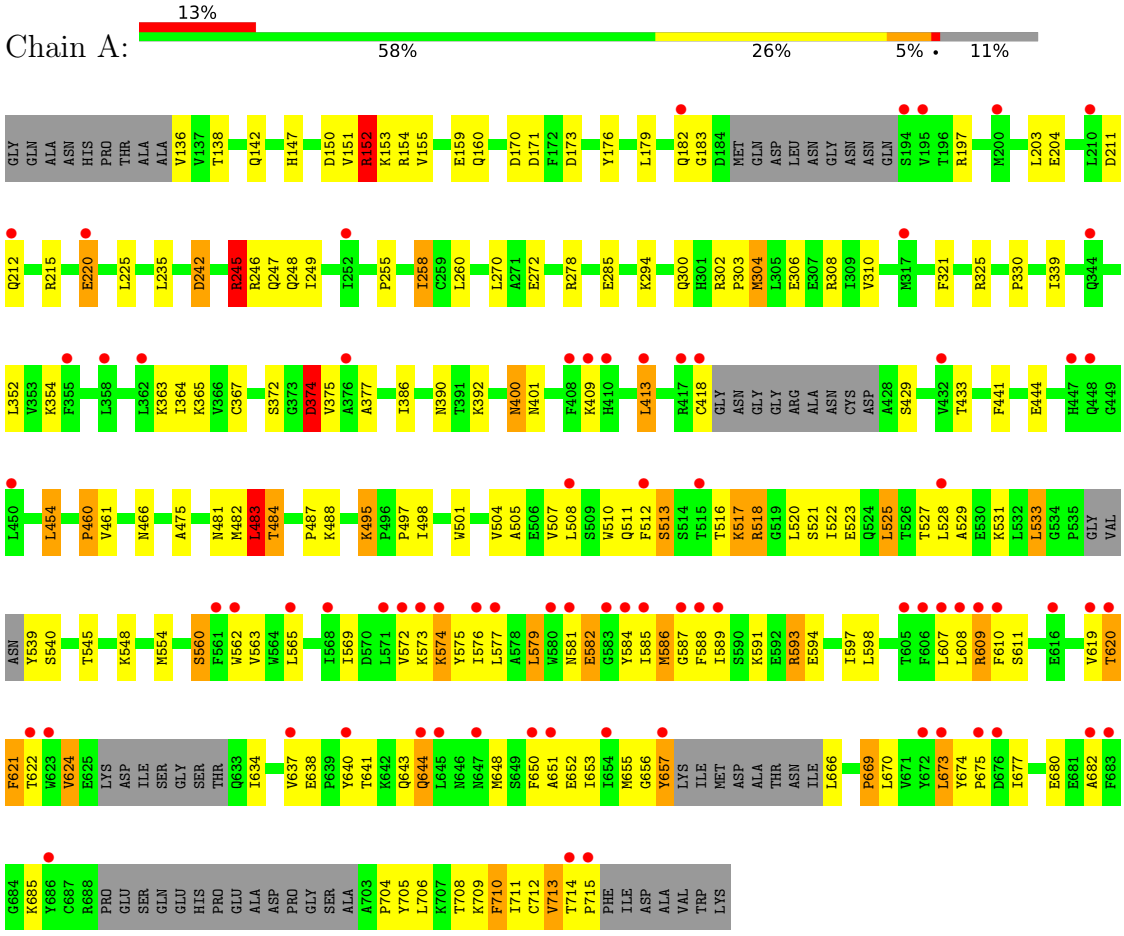
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	6	Total O 6 6	0	0
4	D	5	Total O 5 5	0	0

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.

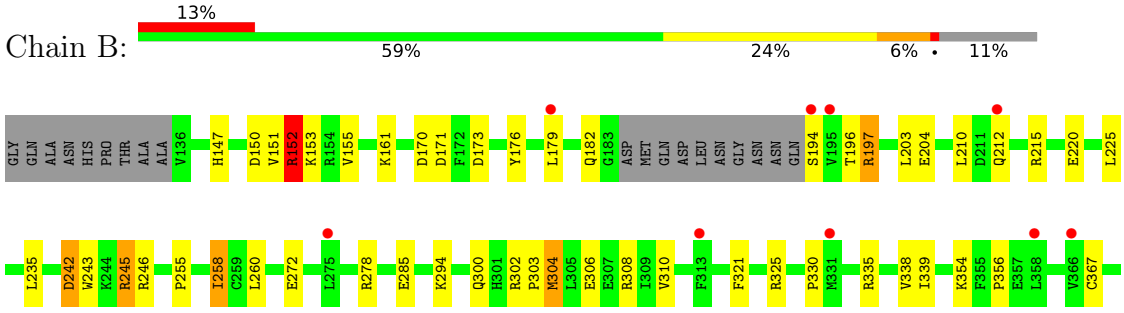
• Molecule 1: Signal transducer and activator of transcription 3

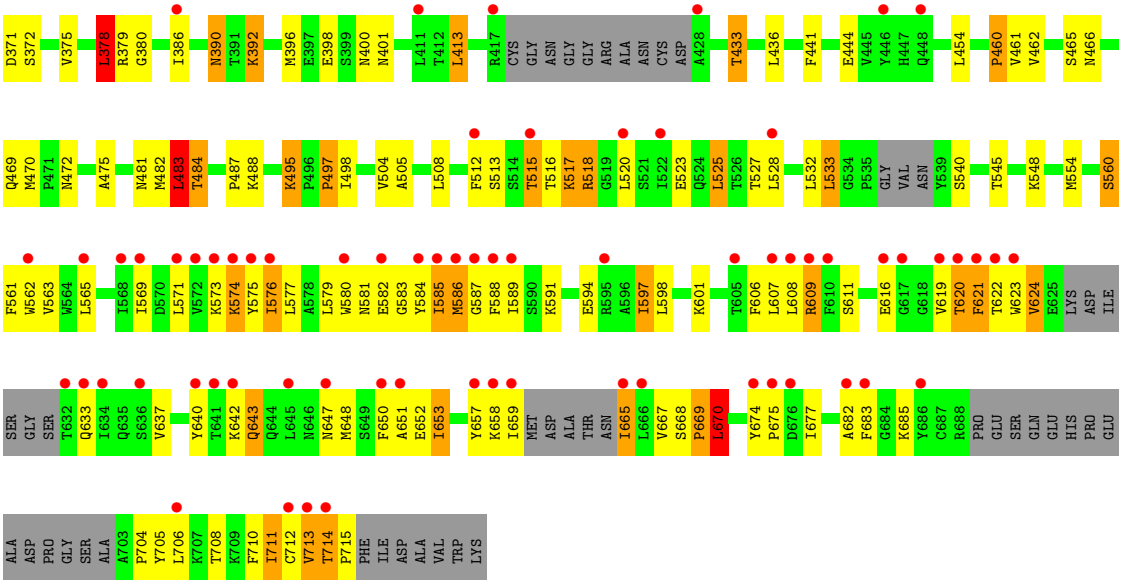
Chain A:



• Molecule 1: Signal transducer and activator of transcription 3

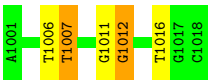
Chain B:





• Molecule 2: DNA (5'-D(*AP*AP*GP*AP*TP*TP*TP*AP*CP*GP*GP*GP*AP*AP*AP*TP *GP*C)-3')

Chain C:



• Molecule 3: DNA (5'-D(*TP*GP*CP*AP*TP*TP*TP*CP*CP*CP*GP*TP*AP*AP*AP*TP *CP*T)-3')

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	175.49Å 175.49Å 79.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 175.49 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.85) 100.0 (175.49-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.294 , 0.343 0.294 , 0.343	Depositor DCC
R_{free} test set	2781 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	75.5	Xtriage
Anisotropy	0.830	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 54.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9454	wwPDB-VP
Average B, all atoms (Å^2)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 98.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.6998e-11. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

Bond lengths and bond angles in the following residue types are not validated in this section: ALY, PTR

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	0.98	2/4364 (0.0%)	1.11	21/5886 (0.4%)
1	B	0.99	2/4374 (0.0%)	1.08	15/5900 (0.3%)
2	C	0.99	1/419 (0.2%)	1.25	4/646 (0.6%)
3	D	0.88	0/401	1.32	7/616 (1.1%)
All	All	0.98	5/9558 (0.1%)	1.12	47/13048 (0.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	272	GLU	CD-OE2	6.47	1.32	1.25
1	B	272	GLU	CD-OE2	6.20	1.32	1.25
1	A	220	GLU	CD-OE1	5.85	1.32	1.25
2	C	1006	DT	O3'-P	-5.57	1.54	1.61
1	B	212	GLN	CG-CD	5.56	1.63	1.51

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1007	DT	O5'-P-OP2	-8.89	97.70	105.70
1	B	152	ARG	NE-CZ-NH1	8.52	124.56	120.30
3	D	1007	DT	O5'-P-OP1	7.88	120.15	110.70
2	C	1012	DG	O5'-P-OP2	-7.19	99.23	105.70
1	A	152	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	B	325	ARG	NE-CZ-NH2	-6.96	116.82	120.30
3	D	1012	DT	O5'-P-OP2	-6.74	99.63	105.70
1	A	170	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	A	171	ASP	CB-CG-OD1	6.15	123.83	118.30
1	B	325	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	483	LEU	CA-CB-CG	6.04	129.18	115.30
3	D	1001	DT	C1'-O4'-C4'	-5.93	104.17	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	378	LEU	CB-CG-CD1	5.91	121.06	111.00
1	A	215	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	B	242	ASP	CB-CG-OD1	5.74	123.47	118.30
1	B	170	ASP	CB-CG-OD2	-5.72	113.15	118.30
3	D	1016	DT	C1'-O4'-C4'	-5.68	104.42	110.10
1	A	242	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	484	THR	CB-CA-C	-5.61	96.45	111.60
1	B	215	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	A	364	ILE	CG1-CB-CG2	-5.58	99.11	111.40
1	B	484	THR	CB-CA-C	-5.58	96.54	111.60
3	D	1015	DA	O5'-P-OP2	5.55	117.36	110.70
1	A	154	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	483	LEU	CA-CB-CG	5.53	128.02	115.30
1	B	171	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	673	LEU	CB-CG-CD2	5.50	120.35	111.00
2	C	1007	DT	O5'-P-OP2	-5.43	100.81	105.70
1	A	560	SER	CB-CA-C	-5.43	99.78	110.10
1	B	560	SER	CB-CA-C	-5.41	99.82	110.10
1	A	325	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	C	1016	DT	N1-C1'-C2'	5.36	122.77	112.60
1	A	278	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	171	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	325	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	A	245	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	B	670	LEU	CB-CG-CD1	5.22	119.88	111.00
2	C	1016	DT	C1'-O4'-C4'	-5.21	104.89	110.10
1	A	593	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	B	278	ARG	NE-CZ-NH2	-5.17	117.72	120.30
3	D	1016	DT	N1-C1'-C2'	5.15	122.39	112.60
1	A	363	LYS	N-CA-CB	-5.14	101.35	110.60
1	B	278	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	454	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	278	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	170	ASP	CB-CG-OD1	5.08	122.88	118.30
1	B	379	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

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	A	4310	0	4367	133	0
1	B	4323	0	4391	136	0
2	C	372	0	204	2	0
3	D	360	0	207	2	0
4	A	42	0	0	2	0
4	B	36	0	0	1	0
4	C	6	0	0	0	0
4	D	5	0	0	0	0
All	All	9454	0	9169	265	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 14.

All (265) 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:A:517:LYS:HE2	1:A:577:LEU:CD2	1.70	1.20
1:A:656:GLY:O	1:A:711:ILE:CD1	1.96	1.13
1:A:711:ILE:HG12	1:A:713:VAL:HG13	1.33	1.10
1:A:517:LYS:HE2	1:A:577:LEU:HD23	1.19	1.09
1:B:505:ALA:HB1	1:B:525:LEU:HD11	1.46	0.96
1:A:711:ILE:CG1	1:A:713:VAL:HG13	1.97	0.94
1:A:656:GLY:O	1:A:711:ILE:HD12	1.67	0.92
1:A:505:ALA:HB1	1:A:525:LEU:HD11	1.49	0.91
1:A:656:GLY:O	1:A:711:ILE:HD11	1.72	0.90
1:A:711:ILE:CD1	1:A:713:VAL:CG1	2.51	0.88
1:A:516:THR:HG22	1:A:577:LEU:HG	1.56	0.87
1:A:656:GLY:C	1:A:711:ILE:CD1	2.44	0.86
1:A:656:GLY:C	1:A:711:ILE:HD12	2.00	0.82
1:A:711:ILE:CD1	1:A:713:VAL:HG13	2.10	0.82
1:A:598:LEU:HG	1:A:624:VAL:HG11	1.62	0.81
1:B:339:ILE:HG21	1:B:413:LEU:HD22	1.67	0.76
1:B:711:ILE:HB	1:B:713:VAL:HG13	1.67	0.76
1:A:585:ILE:HG12	1:A:608:LEU:HD12	1.70	0.74
1:A:339:ILE:HG21	1:A:413:LEU:HD22	1.68	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:ILE:HD11	1:A:713:VAL:CG1	2.20	0.72
1:A:260:LEU:HD22	1:A:352:LEU:HD21	1.70	0.72
1:A:517:LYS:HE2	1:A:577:LEU:HD21	1.67	0.72
1:A:666:LEU:HD11	1:B:665:ILE:HD11	1.71	0.71
1:A:585:ILE:HG12	1:A:608:LEU:CD1	2.19	0.71
1:B:584:TYR:CE2	1:B:682:ALA:HB1	2.26	0.71
1:A:656:GLY:C	1:A:711:ILE:HD11	2.08	0.70
1:A:711:ILE:HD11	1:A:713:VAL:HG12	1.74	0.69
1:A:584:TYR:CE2	1:A:682:ALA:HB1	2.29	0.68
1:A:579:LEU:HD23	1:A:651:ALA:HB2	1.74	0.68
1:B:579:LEU:HD23	1:B:651:ALA:HB2	1.76	0.68
1:B:658:LYS:HB2	1:B:667:VAL:HB	1.75	0.67
1:A:517:LYS:CE	1:A:577:LEU:HD23	2.12	0.66
1:B:579:LEU:HD12	1:B:579:LEU:H	1.61	0.66
1:A:710:PHE:HB3	1:B:712:CYS:N	2.11	0.66
1:A:579:LEU:H	1:A:579:LEU:HD12	1.62	0.65
1:B:576:ILE:HA	1:B:579:LEU:HD13	1.78	0.65
1:A:516:THR:CG2	1:A:577:LEU:HG	2.25	0.65
1:A:245:ARG:NH1	1:A:481:ASN:O	2.31	0.64
1:B:582:GLU:HB3	1:B:584:TYR:CD1	2.33	0.63
1:A:597:ILE:HD12	1:A:622:THR:HG21	1.79	0.63
1:B:465:SER:H	1:B:469:GLN:HE22	1.45	0.63
1:B:197:ARG:HB3	1:B:197:ARG:HH21	1.62	0.63
1:A:574:LYS:O	1:A:574:LYS:HD3	1.97	0.63
1:B:245:ARG:NH1	1:B:481:ASN:O	2.31	0.63
1:A:152:ARG:HG3	1:A:152:ARG:HH11	1.63	0.63
1:B:152:ARG:HH11	1:B:152:ARG:HG3	1.63	0.63
1:B:243:TRP:CE2	1:B:260:LEU:HD21	2.34	0.63
1:A:657:TYR:HA	1:A:713:VAL:HG12	1.80	0.63
1:B:225:LEU:HD13	1:B:308:ARG:HB2	1.81	0.63
1:A:714:THR:N	1:A:715:PRO:HD2	2.13	0.63
1:A:576:ILE:HA	1:A:579:LEU:HD13	1.81	0.62
1:B:147:HIS:O	1:B:151:VAL:HG23	1.98	0.62
1:B:659:ILE:HG13	1:B:714:THR:HG21	1.82	0.62
1:A:147:HIS:O	1:A:151:VAL:HG23	2.00	0.61
1:B:512:PHE:CE2	1:B:520:LEU:HD21	2.35	0.61
1:B:580:TRP:HA	1:B:585:ILE:HG13	1.81	0.61
1:A:225:LEU:HD13	1:A:308:ARG:HB2	1.83	0.61
1:A:598:LEU:CG	1:A:624:VAL:HG11	2.29	0.61
1:A:609:ARG:HH11	1:A:620:THR:HG21	1.65	0.61
1:A:585:ILE:HG23	1:A:608:LEU:CB	2.31	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:ARG:HH21	1:B:620:THR:HG21	1.66	0.60
3:D:1001:DT:H2'	3:D:1002:DG:C8	2.36	0.60
1:A:339:ILE:HD12	1:A:461:VAL:HG11	1.82	0.60
1:B:516:THR:HG22	1:B:577:LEU:HG	1.84	0.60
1:A:711:ILE:HG12	1:A:713:VAL:CG1	2.23	0.59
1:A:545:THR:HG23	1:A:548:LYS:H	1.68	0.59
1:B:571:LEU:HD13	1:B:642:LYS:HE2	1.85	0.59
1:A:179:LEU:HD12	1:A:203:LEU:HD22	1.85	0.58
1:A:512:PHE:CE2	1:A:520:LEU:HD21	2.38	0.58
1:B:586:MET:CB	1:B:607:LEU:HD11	2.33	0.58
1:B:585:ILE:HG23	1:B:608:LEU:HB2	1.85	0.58
1:A:585:ILE:HG23	1:A:608:LEU:HB2	1.84	0.58
1:A:641:THR:HG23	1:A:644:GLN:H	1.69	0.58
1:B:367:CYS:HA	1:B:386:ILE:HD12	1.86	0.57
1:B:498:ILE:HD12	1:B:545:THR:HG22	1.86	0.57
1:B:338:VAL:HG11	1:B:470:MET:CE	2.34	0.57
1:B:517:LYS:CD	1:B:517:LYS:H	2.16	0.57
1:B:517:LYS:H	1:B:517:LYS:HD3	1.69	0.57
1:A:711:ILE:HD13	1:A:713:VAL:CG1	2.32	0.57
1:A:517:LYS:H	1:A:517:LYS:HD3	1.68	0.56
1:A:306:GLU:O	1:A:310:VAL:HG23	2.05	0.56
1:B:643:GLN:O	1:B:643:GLN:HG3	2.04	0.56
1:A:527:THR:HG21	1:A:589:ILE:CA	2.35	0.56
1:B:306:GLU:O	1:B:310:VAL:HG23	2.06	0.56
1:A:516:THR:HG22	1:A:577:LEU:CG	2.30	0.55
1:B:354:LYS:NZ	1:B:401:ASN:O	2.40	0.55
1:B:714:THR:OG1	1:B:715:PRO:HD2	2.06	0.55
1:B:657:TYR:HA	1:B:713:VAL:HG12	1.87	0.55
1:B:623:TRP:CD1	1:B:623:TRP:N	2.75	0.55
1:A:584:TYR:HE2	1:A:682:ALA:O	1.90	0.55
1:B:623:TRP:HB3	1:B:670:LEU:HD23	1.88	0.55
1:A:248:GLN:HB2	4:A:802:HOH:O	2.07	0.54
1:B:597:ILE:HD11	1:B:622:THR:HG21	1.89	0.54
1:A:367:CYS:HA	1:A:386:ILE:HD12	1.88	0.54
1:A:533:LEU:N	1:A:533:LEU:HD22	2.23	0.54
1:B:523:GLU:OE2	1:B:523:GLU:N	2.29	0.53
1:A:151:VAL:O	1:A:155:VAL:HG23	2.09	0.53
1:A:138:THR:O	1:A:142:GLN:HG3	2.08	0.53
1:B:581:ASN:C	1:B:583:GLY:H	2.11	0.53
1:B:582:GLU:HB3	1:B:584:TYR:CE1	2.43	0.53
1:B:197:ARG:HB3	1:B:197:ARG:NH2	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:650:PHE:HA	1:B:653:ILE:HG22	1.89	0.53
1:B:151:VAL:O	1:B:155:VAL:HG23	2.08	0.53
1:B:587:GLY:HA2	1:B:609:ARG:HA	1.91	0.53
1:B:533:LEU:N	1:B:533:LEU:HD22	2.24	0.52
1:A:710:PHE:HB3	1:B:712:CYS:CA	2.39	0.52
1:B:648:MET:HG2	1:B:652:GLU:HB3	1.91	0.52
1:B:339:ILE:HD12	1:B:461:VAL:HG11	1.90	0.52
1:A:374:ASP:H	1:A:377:ALA:HB3	1.73	0.52
1:B:591:LYS:HA	1:B:594:GLU:HB3	1.91	0.52
1:A:517:LYS:HE3	1:A:581:ASN:HB2	1.90	0.52
1:A:588:PHE:CE1	1:A:610:PHE:HD2	2.27	0.52
1:B:285:GLU:HB2	1:B:302:ARG:HD2	1.92	0.52
1:A:587:GLY:HA2	1:A:609:ARG:HA	1.92	0.51
1:A:285:GLU:HB2	1:A:302:ARG:HD2	1.92	0.51
1:A:517:LYS:HD3	1:A:517:LYS:N	2.25	0.51
1:B:597:ILE:CD1	1:B:622:THR:HG21	2.41	0.51
1:A:504:VAL:HG12	1:A:508:LEU:CD1	2.41	0.51
1:A:650:PHE:HA	1:A:653:ILE:HG22	1.91	0.51
1:B:504:VAL:HG12	1:B:508:LEU:CD1	2.41	0.51
1:A:527:THR:HG21	1:A:589:ILE:N	2.25	0.50
1:A:582:GLU:HB3	1:A:584:TYR:CD1	2.47	0.50
2:C:1011:DG:H2"	2:C:1012:DG:C8	2.46	0.50
1:A:648:MET:HG2	1:A:652:GLU:HB3	1.92	0.50
1:B:466:ASN:ND2	2:C:1007:DT:O4	2.44	0.50
1:A:517:LYS:H	1:A:517:LYS:CD	2.23	0.50
1:A:354:LYS:NZ	1:A:401:ASN:O	2.39	0.49
1:B:475:ALA:HB2	1:B:562:TRP:CD1	2.48	0.49
1:B:584:TYR:HE2	1:B:682:ALA:O	1.96	0.49
1:A:475:ALA:HB2	1:A:562:TRP:CD1	2.47	0.49
1:A:644:GLN:HA	1:A:644:GLN:HE21	1.77	0.49
1:B:585:ILE:HG23	1:B:608:LEU:CB	2.42	0.49
1:B:390:ASN:H	1:B:390:ASN:HD22	1.60	0.48
1:A:249:ILE:HG13	4:A:802:HOH:O	2.12	0.48
1:A:339:ILE:CG2	1:A:413:LEU:HD22	2.42	0.48
1:B:378:LEU:HD12	1:B:380:GLY:H	1.77	0.48
1:B:338:VAL:HG11	1:B:470:MET:HE2	1.95	0.48
1:B:339:ILE:CG2	1:B:413:LEU:HD22	2.41	0.48
1:A:711:ILE:CG1	1:A:713:VAL:CG1	2.78	0.48
1:B:465:SER:H	1:B:469:GLN:NE2	2.10	0.48
1:A:598:LEU:CD2	1:A:624:VAL:HG11	2.44	0.48
1:B:243:TRP:CD2	1:B:260:LEU:HD21	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:TRP:CZ2	1:B:260:LEU:HD21	2.48	0.48
1:B:598:LEU:HD13	1:B:598:LEU:HA	1.70	0.48
1:B:523:GLU:H	1:B:523:GLU:CD	2.15	0.48
1:B:569:ILE:HG22	1:B:569:ILE:O	2.12	0.48
1:B:304:MET:SD	1:B:308:ARG:NH1	2.87	0.47
1:B:528:LEU:HD11	1:B:588:PHE:CE2	2.50	0.47
1:A:518:ARG:HD2	1:A:581:ASN:HA	1.95	0.47
1:A:585:ILE:HG12	1:A:608:LEU:HD13	1.96	0.47
1:A:365:LYS:HE2	1:A:390:ASN:ND2	2.29	0.47
1:A:517:LYS:CE	1:A:581:ASN:HB2	2.44	0.47
1:A:586:MET:CB	1:A:607:LEU:HD11	2.44	0.47
1:B:606:PHE:CE2	1:B:683:PHE:HE2	2.33	0.47
1:A:482:MET:HG2	1:A:483:LEU:HD13	1.96	0.47
1:A:594:GLU:O	1:A:597:ILE:HG12	2.15	0.47
1:B:609:ARG:HB3	1:B:620:THR:HG22	1.97	0.47
1:A:574:LYS:HB3	1:A:575:TYR:CD1	2.49	0.47
1:B:441:PHE:CD1	1:B:441:PHE:N	2.83	0.47
1:B:504:VAL:HG12	1:B:508:LEU:HD11	1.97	0.46
1:B:515:THR:HG23	1:B:573:LYS:HD3	1.97	0.46
1:A:304:MET:SD	1:A:308:ARG:NH2	2.88	0.46
1:A:504:VAL:HG12	1:A:508:LEU:HD11	1.97	0.46
1:A:657:TYR:HD1	1:A:657:TYR:O	1.97	0.46
1:A:152:ARG:HG3	1:A:152:ARG:NH1	2.29	0.46
1:A:242:ASP:O	1:A:246:ARG:HG3	2.15	0.46
1:B:647:ASN:N	1:B:647:ASN:ND2	2.62	0.46
1:A:375:VAL:O	1:A:375:VAL:HG13	2.15	0.46
1:B:581:ASN:C	1:B:583:GLY:N	2.67	0.46
1:A:531:LYS:NZ	1:A:554:MET:CE	2.79	0.46
1:B:242:ASP:O	1:B:246:ARG:HG3	2.16	0.46
1:B:482:MET:HG2	1:B:483:LEU:HD13	1.98	0.46
1:A:510:TRP:HA	1:A:513:SER:HB2	1.98	0.45
1:A:579:LEU:H	1:A:579:LEU:CD1	2.28	0.45
1:A:304:MET:O	1:A:308:ARG:HG2	2.16	0.45
1:B:176:TYR:HA	1:B:203:LEU:HD21	1.98	0.45
1:B:579:LEU:H	1:B:579:LEU:CD1	2.28	0.45
1:B:647:ASN:N	1:B:647:ASN:HD22	2.12	0.45
1:A:466:ASN:ND2	3:D:1007:DT:O4	2.47	0.45
1:B:515:THR:HG23	1:B:516:THR:HG23	1.99	0.45
1:B:527:THR:HG21	1:B:589:ILE:N	2.32	0.45
1:A:609:ARG:HB3	1:A:620:THR:HG22	1.98	0.45
1:B:304:MET:O	1:B:308:ARG:HG2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:PHE:N	1:A:441:PHE:CD1	2.84	0.45
1:B:517:LYS:HZ2	1:B:581:ASN:HB2	1.81	0.45
1:B:606:PHE:HE2	1:B:683:PHE:CE2	2.35	0.45
1:B:152:ARG:HG3	1:B:152:ARG:NH1	2.29	0.45
1:B:518:ARG:NH1	1:B:581:ASN:O	2.50	0.45
1:A:523:GLU:CD	1:A:523:GLU:H	2.20	0.45
1:A:569:ILE:O	1:A:572:VAL:HG22	2.17	0.45
1:A:577:LEU:HD23	1:A:577:LEU:O	2.17	0.45
1:A:591:LYS:HA	1:A:594:GLU:HB3	1.99	0.45
1:A:708:THR:HB	1:B:712:CYS:SG	2.57	0.45
1:B:433:THR:HG21	1:B:472:ASN:HB3	1.99	0.45
1:B:466:ASN:H	1:B:469:GLN:NE2	2.14	0.45
1:A:657:TYR:CA	1:A:711:ILE:HD11	2.47	0.45
1:B:586:MET:HB3	1:B:607:LEU:HD11	1.99	0.45
1:A:528:LEU:HD11	1:A:588:PHE:CE2	2.52	0.44
1:B:598:LEU:HG	1:B:624:VAL:HG11	2.00	0.44
1:B:460:PRO:HD3	1:B:487:PRO:O	2.18	0.44
1:A:460:PRO:HD3	1:A:487:PRO:O	2.18	0.44
1:B:598:LEU:HD11	1:B:624:VAL:HG21	2.00	0.44
1:B:371:ASP:HB3	1:B:375:VAL:HG11	1.99	0.44
1:B:658:LYS:O	1:B:713:VAL:HB	2.18	0.44
1:B:706:LEU:HD23	1:B:706:LEU:HA	1.75	0.44
1:A:512:PHE:CD2	1:A:520:LEU:HD21	2.52	0.43
1:A:518:ARG:HB3	1:A:581:ASN:HB3	1.99	0.43
1:A:176:TYR:HA	1:A:203:LEU:HD21	2.01	0.43
1:B:606:PHE:HB3	1:B:670:LEU:HD22	2.01	0.43
1:B:580:TRP:CZ3	1:B:585:ILE:HB	2.53	0.43
1:A:495:LYS:HD2	1:A:495:LYS:O	2.19	0.43
1:A:712:CYS:CB	1:B:710:PHE:HB3	2.48	0.43
1:B:356:PRO:HA	1:B:396:MET:CE	2.49	0.43
1:B:579:LEU:HD12	1:B:579:LEU:N	2.31	0.43
1:B:258:ILE:HA	1:B:258:ILE:HD12	1.74	0.43
1:B:571:LEU:HD12	1:B:571:LEU:HA	1.86	0.43
1:A:507:VAL:O	1:A:511:GLN:HG2	2.18	0.43
1:B:505:ALA:HA	1:B:508:LEU:HD12	2.01	0.43
1:B:392:LYS:HB2	1:B:392:LYS:HE2	1.66	0.43
1:B:569:ILE:O	1:B:569:ILE:CG2	2.66	0.43
1:B:577:LEU:HD23	1:B:577:LEU:O	2.19	0.43
1:A:517:LYS:NZ	1:A:581:ASN:HB2	2.34	0.43
1:A:621:PHE:O	1:A:621:PHE:HD1	2.02	0.43
1:B:338:VAL:CG1	1:B:470:MET:CE	2.96	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:TYR:HA	1:A:711:ILE:HD11	2.00	0.42
1:B:321:PHE:HB2	1:B:454:LEU:HD13	2.01	0.42
1:B:598:LEU:CD1	1:B:624:VAL:HG21	2.49	0.42
1:A:585:ILE:HG23	1:A:608:LEU:HB3	2.00	0.42
1:B:674:TYR:CD1	1:B:674:TYR:C	2.92	0.42
1:B:607:LEU:O	1:B:621:PHE:HA	2.19	0.42
1:A:674:TYR:CD1	1:A:674:TYR:C	2.93	0.42
1:B:574:LYS:HB3	1:B:575:TYR:CD1	2.55	0.42
1:A:321:PHE:HB2	1:A:454:LEU:HD13	2.02	0.42
1:A:400:ASN:ND2	1:A:400:ASN:H	2.15	0.42
1:A:598:LEU:HD13	1:A:598:LEU:HA	1.77	0.42
1:B:495:LYS:CD	1:B:495:LYS:O	2.67	0.42
1:B:495:LYS:O	1:B:495:LYS:HD2	2.20	0.42
1:B:554:MET:SD	1:B:561:PHE:HA	2.60	0.42
1:A:495:LYS:O	1:A:495:LYS:CD	2.68	0.42
1:B:601:LYS:HE3	1:B:674:TYR:CE2	2.55	0.42
1:B:210:LEU:HD12	1:B:210:LEU:HA	1.87	0.42
1:A:560:SER:HB2	1:A:563:VAL:HB	2.02	0.41
1:A:527:THR:HG21	1:A:589:ILE:HA	2.01	0.41
1:B:585:ILE:HG22	1:B:587:GLY:N	2.36	0.41
1:B:609:ARG:O	1:B:620:THR:N	2.53	0.41
1:B:335:ARG:NH1	4:B:801:HOH:O	2.54	0.41
1:B:571:LEU:HD11	1:B:642:LYS:HG2	2.02	0.41
1:A:247:GLN:HA	1:A:258:ILE:HD11	2.03	0.41
1:A:302:ARG:N	1:A:303:PRO:CD	2.84	0.41
1:A:505:ALA:HA	1:A:508:LEU:HD12	2.03	0.41
1:B:532:LEU:HD23	1:B:532:LEU:HA	1.76	0.41
1:B:302:ARG:N	1:B:303:PRO:CD	2.83	0.41
1:B:621:PHE:HD1	1:B:621:PHE:O	2.04	0.41
1:B:659:ILE:HB	1:B:714:THR:HB	2.02	0.41
1:B:518:ARG:H	1:B:581:ASN:ND2	2.19	0.41
1:B:606:PHE:HE2	1:B:683:PHE:HE2	1.69	0.41
1:A:712:CYS:HA	1:B:710:PHE:HB3	2.04	0.40
1:B:436:LEU:HD23	1:B:462:VAL:HG22	2.03	0.40
1:B:560:SER:HB2	1:B:563:VAL:HB	2.02	0.40
1:A:501:TRP:CZ2	1:A:529:ALA:HB2	2.56	0.40
1:A:539:TYR:CD1	1:A:539:TYR:N	2.89	0.40
1:A:588:PHE:CE1	1:A:610:PHE:CD2	3.08	0.40
1:B:512:PHE:CD2	1:B:520:LEU:HD21	2.56	0.40
1:B:606:PHE:CE2	1:B:683:PHE:CE2	3.10	0.40
1:A:706:LEU:HD23	1:A:706:LEU:HA	1.80	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	515/596 (86%)	488 (95%)	20 (4%)	7 (1%)	11 31
1	B	516/596 (87%)	485 (94%)	23 (4%)	8 (2%)	9 28
All	All	1031/1192 (86%)	973 (94%)	43 (4%)	15 (2%)	10 30

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	GLY
1	A	669	PRO
1	A	704	PRO
1	B	497	PRO
1	B	669	PRO
1	B	704	PRO
1	A	497	PRO
1	A	374	ASP
1	A	713	VAL
1	B	378	LEU
1	B	713	VAL
1	B	540	SER
1	B	668	SER
1	B	675	PRO
1	A	675	PRO

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	483/532 (91%)	409 (85%)	74 (15%)	2 7
1	B	484/532 (91%)	418 (86%)	66 (14%)	3 9
All	All	967/1064 (91%)	827 (86%)	140 (14%)	3 8

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	VAL
1	A	150	ASP
1	A	152	ARG
1	A	153	LYS
1	A	159	GLU
1	A	160	GLN
1	A	173	ASP
1	A	182	GLN
1	A	197	ARG
1	A	204	GLU
1	A	211	ASP
1	A	212	GLN
1	A	220	GLU
1	A	235	LEU
1	A	245	ARG
1	A	255	PRO
1	A	258	ILE
1	A	270	LEU
1	A	294	LYS
1	A	300	GLN
1	A	304	MET
1	A	330	PRO
1	A	372	SER
1	A	374	ASP
1	A	392	LYS
1	A	400	ASN
1	A	409	LYS
1	A	413	LEU
1	A	418	CYS
1	A	429	SER
1	A	433	THR
1	A	444	GLU
1	A	460	PRO
1	A	483	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	484	THR
1	A	488	LYS
1	A	495	LYS
1	A	498	ILE
1	A	513	SER
1	A	517	LYS
1	A	518	ARG
1	A	521	SER
1	A	522	ILE
1	A	525	LEU
1	A	533	LEU
1	A	540	SER
1	A	565	LEU
1	A	573	LYS
1	A	574	LYS
1	A	579	LEU
1	A	582	GLU
1	A	586	MET
1	A	593	ARG
1	A	609	ARG
1	A	611	SER
1	A	619	VAL
1	A	620	THR
1	A	621	PHE
1	A	624	VAL
1	A	634	ILE
1	A	637	VAL
1	A	638	GLU
1	A	640	TYR
1	A	643	GLN
1	A	644	GLN
1	A	655	MET
1	A	657	TYR
1	A	669	PRO
1	A	670	LEU
1	A	673	LEU
1	A	677	ILE
1	A	680	GLU
1	A	709	LYS
1	A	710	PHE
1	B	150	ASP
1	B	152	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	153	LYS
1	B	161	LYS
1	B	173	ASP
1	B	179	LEU
1	B	182	GLN
1	B	194	SER
1	B	196	THR
1	B	197	ARG
1	B	204	GLU
1	B	220	GLU
1	B	235	LEU
1	B	245	ARG
1	B	255	PRO
1	B	258	ILE
1	B	294	LYS
1	B	300	GLN
1	B	304	MET
1	B	330	PRO
1	B	372	SER
1	B	390	ASN
1	B	392	LYS
1	B	398	GLU
1	B	400	ASN
1	B	413	LEU
1	B	433	THR
1	B	444	GLU
1	B	460	PRO
1	B	483	LEU
1	B	484	THR
1	B	488	LYS
1	B	495	LYS
1	B	497	PRO
1	B	513	SER
1	B	515	THR
1	B	517	LYS
1	B	518	ARG
1	B	525	LEU
1	B	533	LEU
1	B	548	LYS
1	B	565	LEU
1	B	574	LYS
1	B	576	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	585	ILE
1	B	586	MET
1	B	597	ILE
1	B	609	ARG
1	B	611	SER
1	B	616	GLU
1	B	619	VAL
1	B	620	THR
1	B	621	PHE
1	B	624	VAL
1	B	633	GLN
1	B	637	VAL
1	B	640	TYR
1	B	643	GLN
1	B	653	ILE
1	B	665	ILE
1	B	669	PRO
1	B	670	LEU
1	B	677	ILE
1	B	708	THR
1	B	711	ILE
1	B	714	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	GLN
1	A	212	GLN
1	A	315	ASN
1	A	344	GLN
1	A	457	HIS
1	A	472	ASN
1	A	567	ASN
1	A	644	GLN
1	B	205	GLN
1	B	315	ASN
1	B	344	GLN
1	B	390	ASN
1	B	448	GLN
1	B	457	HIS
1	B	469	GLN
1	B	543	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	567	ASN
1	B	581	ASN
1	B	647	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	ALY	B	685	1	10,11,12	0.80	0	7,12,14	2.40	4 (57%)
1	PTR	B	705	1	15,16,17	2.61	7 (46%)	19,22,24	2.30	7 (36%)
1	PTR	A	705	1	15,16,17	2.70	8 (53%)	19,22,24	1.96	4 (21%)
1	ALY	A	685	1	10,11,12	0.87	0	7,12,14	2.22	3 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ALY	B	685	1	-	3/9/10/12	-
1	PTR	B	705	1	-	4/10/11/13	0/1/1/1
1	PTR	A	705	1	-	1/10/11/13	0/1/1/1
1	ALY	A	685	1	-	3/9/10/12	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	705	PTR	CE1-CD1	4.71	1.47	1.38
1	B	705	PTR	CE2-CD2	4.67	1.47	1.38
1	A	705	PTR	CE2-CD2	4.46	1.46	1.38
1	B	705	PTR	CE1-CD1	4.36	1.46	1.38
1	A	705	PTR	OH-CZ	4.04	1.49	1.40
1	B	705	PTR	CE1-CZ	3.87	1.46	1.38
1	A	705	PTR	P-OH	3.60	1.64	1.59
1	B	705	PTR	OH-CZ	3.29	1.48	1.40
1	A	705	PTR	CE1-CZ	3.22	1.45	1.38
1	B	705	PTR	CE2-CZ	3.18	1.45	1.38
1	B	705	PTR	CB-CG	3.16	1.58	1.51
1	A	705	PTR	CB-CG	2.99	1.58	1.51
1	B	705	PTR	CD2-CG	2.74	1.44	1.38
1	A	705	PTR	CD2-CG	2.63	1.44	1.38
1	A	705	PTR	CE2-CZ	2.58	1.43	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	705	PTR	CE2-CZ-CE1	-4.69	112.95	120.18
1	B	705	PTR	CG-CB-CA	4.49	123.20	114.10
1	B	705	PTR	CD1-CE1-CZ	4.21	124.88	119.73
1	A	705	PTR	CG-CB-CA	4.02	122.23	114.10
1	A	705	PTR	CE2-CZ-CE1	-3.82	114.30	120.18
1	B	685	ALY	CD-CE-NZ	3.60	122.51	112.21
1	A	705	PTR	CD1-CE1-CZ	3.58	124.11	119.73
1	A	685	ALY	CD-CE-NZ	3.38	121.86	112.21
1	A	685	ALY	CH3-CH-NZ	3.28	121.91	116.09
1	B	685	ALY	CH3-CH-NZ	3.24	121.83	116.09
1	B	705	PTR	CB-CG-CD2	2.86	126.58	120.91
1	B	685	ALY	CG-CD-CE	-2.80	100.29	113.56
1	A	705	PTR	CB-CG-CD2	2.52	125.91	120.91
1	B	705	PTR	O3P-P-O2P	2.50	117.20	107.64
1	A	685	ALY	CG-CD-CE	-2.49	101.75	113.56
1	B	685	ALY	OH-CH-CH3	-2.10	118.16	122.06
1	B	705	PTR	OH-CZ-CE1	2.08	125.43	119.23
1	B	705	PTR	CD2-CE2-CZ	2.02	122.21	119.73

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	705	PTR	O-C-CA-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	B	705	PTR	O-C-CA-CB
1	A	685	ALY	OH-CH-NZ-CE
1	A	685	ALY	CH3-CH-NZ-CE
1	B	685	ALY	OH-CH-NZ-CE
1	B	685	ALY	CH3-CH-NZ-CE
1	A	685	ALY	CG-CD-CE-NZ
1	B	705	PTR	CA-CB-CG-CD1
1	B	705	PTR	CA-CB-CG-CD2
1	B	705	PTR	CZ-OH-P-O3P
1	B	685	ALY	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

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	A	528/596 (88%)	0.84	75 (14%) 2 2	70, 100, 170, 194	0
1	B	530/596 (88%)	0.84	77 (14%) 2 1	71, 100, 173, 225	0
2	C	18/18 (100%)	0.09	0 100 100	76, 92, 115, 119	0
3	D	18/18 (100%)	0.07	0 100 100	72, 89, 112, 116	0
All	All	1094/1228 (89%)	0.81	152 (13%) 2 2	70, 99, 171, 225	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	650	PHE	13.4
1	B	650	PHE	9.3
1	A	589	ILE	7.1
1	B	665	ILE	6.5
1	A	418	CYS	6.5
1	A	623	TRP	6.5
1	B	580	TRP	6.5
1	B	622	THR	6.4
1	B	676	ASP	5.9
1	A	608	LEU	5.7
1	A	605	THR	5.6
1	A	417	ARG	5.5
1	A	573	LYS	5.5
1	B	195	VAL	5.5
1	A	651	ALA	5.1
1	A	714	THR	5.1
1	B	651	ALA	5.1
1	B	574	LYS	5.1
1	B	610	PHE	5.1
1	B	640	TYR	5.1
1	A	610	PHE	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	572	VAL	5.0
1	B	584	TYR	4.9
1	B	623	TRP	4.8
1	B	573	LYS	4.7
1	A	584	TYR	4.7
1	A	609	ARG	4.6
1	B	619	VAL	4.6
1	B	588	PHE	4.6
1	A	588	PHE	4.4
1	A	676	ASP	4.3
1	B	666	LEU	4.3
1	B	428	ALA	4.2
1	A	583	GLY	4.2
1	B	212	GLN	4.1
1	B	659	ILE	4.1
1	B	683	PHE	4.1
1	A	622	THR	4.1
1	B	605	THR	4.0
1	A	619	VAL	4.0
1	A	576	ILE	4.0
1	B	609	ARG	3.9
1	A	607	LEU	3.9
1	A	512	PHE	3.8
1	A	647	ASN	3.8
1	A	568	ILE	3.8
1	B	569	ILE	3.7
1	B	657	TYR	3.7
1	A	657	TYR	3.7
1	B	620	THR	3.7
1	A	574	LYS	3.7
1	B	686	TYR	3.7
1	B	515	THR	3.6
1	B	607	LEU	3.5
1	B	621	PHE	3.5
1	A	447	HIS	3.5
1	B	589	ILE	3.5
1	B	512	PHE	3.4
1	A	195	VAL	3.4
1	B	608	LEU	3.4
1	A	580	TRP	3.3
1	B	645	LEU	3.3
1	A	587	GLY	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	644	GLN	3.2
1	B	194	SER	3.2
1	B	682	ALA	3.2
1	A	672	TYR	3.1
1	A	715	PRO	3.1
1	A	212	GLN	3.1
1	A	376	ALA	3.1
1	A	640	TYR	3.0
1	A	637	VAL	3.0
1	B	675	PRO	3.0
1	A	448	GLN	3.0
1	B	358	LEU	3.0
1	A	515	THR	3.0
1	B	586	MET	3.0
1	B	658	LYS	2.9
1	B	417	ARG	2.9
1	B	647	ASN	2.9
1	B	585	ILE	2.9
1	B	616	GLU	2.8
1	B	386	ILE	2.8
1	B	576	ILE	2.8
1	A	686	TYR	2.7
1	B	520	LEU	2.7
1	A	577	LEU	2.7
1	A	673	LEU	2.6
1	B	572	VAL	2.6
1	B	641	THR	2.6
1	A	654	ILE	2.6
1	A	683	PHE	2.6
1	A	565	LEU	2.6
1	A	528	LEU	2.6
1	B	642	LYS	2.6
1	B	587	GLY	2.6
1	A	616	GLU	2.6
1	B	634	ILE	2.6
1	A	585	ILE	2.5
1	B	706	LEU	2.5
1	B	714	THR	2.5
1	B	633	GLN	2.4
1	A	358	LEU	2.4
1	A	562	TRP	2.4
1	A	682	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	355	PHE	2.4
1	B	575	TYR	2.4
1	B	179	LEU	2.4
1	B	528	LEU	2.4
1	B	313	PHE	2.4
1	B	712	CYS	2.4
1	A	182	GLN	2.3
1	A	581	ASN	2.3
1	B	446	TYR	2.3
1	A	620	THR	2.3
1	A	645	LEU	2.3
1	B	568	ILE	2.3
1	B	562	TRP	2.3
1	B	448	GLN	2.3
1	B	366	VAL	2.3
1	B	522	ILE	2.3
1	B	632	THR	2.3
1	A	508	LEU	2.3
1	A	252	ILE	2.2
1	A	606	PHE	2.2
1	A	571	LEU	2.2
1	B	411	LEU	2.2
1	A	409	LYS	2.2
1	B	582	GLU	2.2
1	A	317	MET	2.2
1	A	675	PRO	2.2
1	A	561	PHE	2.1
1	A	408	PHE	2.1
1	A	450	LEU	2.1
1	B	571	LEU	2.1
1	B	636	SER	2.1
1	B	275	LEU	2.1
1	A	200	MET	2.1
1	A	432	VAL	2.1
1	B	713	VAL	2.1
1	A	210	LEU	2.1
1	A	344	GLN	2.1
1	B	617	GLY	2.1
1	A	362	LEU	2.0
1	A	413	LEU	2.0
1	B	565	LEU	2.0
1	A	410	HIS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	194	SER	2.0
1	A	220	GLU	2.0
1	B	674	TYR	2.0
1	B	595	ARG	2.0
1	B	331	MET	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	PTR	A	705	16/17	0.81	0.19	147,157,166,170	0
1	PTR	B	705	16/17	0.82	0.18	153,160,168,173	0
1	ALY	B	685	12/13	0.83	0.29	142,145,146,148	0
1	ALY	A	685	12/13	0.87	0.39	140,144,146,147	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.