Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:31 PM GMT

PDB ID	:	4Y6K
Title	:	Complex structure of presenilin homologue PSH bound to an inhibitor
Authors	:	Dang, S.; Wu, S.; Wang, J.; Shi, Y.
Deposited on	:	2015-02-13
Resolution	:	3.85 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

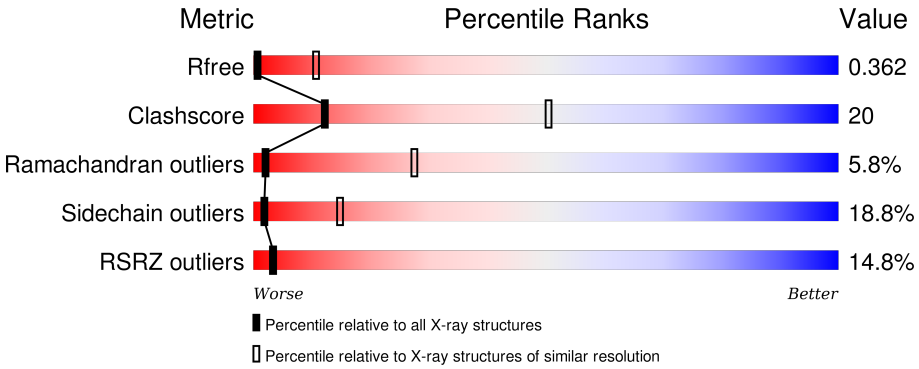
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.85 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}	91344	1000 (4.20-3.52)
Clashscore	102246	1090 (4.20-3.52)
Ramachandran outliers	100387	1046 (4.20-3.52)
Sidechain outliers	100360	1038 (4.20-3.52)
RSRZ outliers	91569	1004 (4.20-3.52)

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. 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	301	12% 39% 35% 7% 18%
1	B	301	15% 43% 30% 7% • 19%
1	C	301	10% 42% 29% 7% • 21%
1	D	301	11% 40% 31% 7% • 21%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	4B5	C	501	-	-	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7200 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.

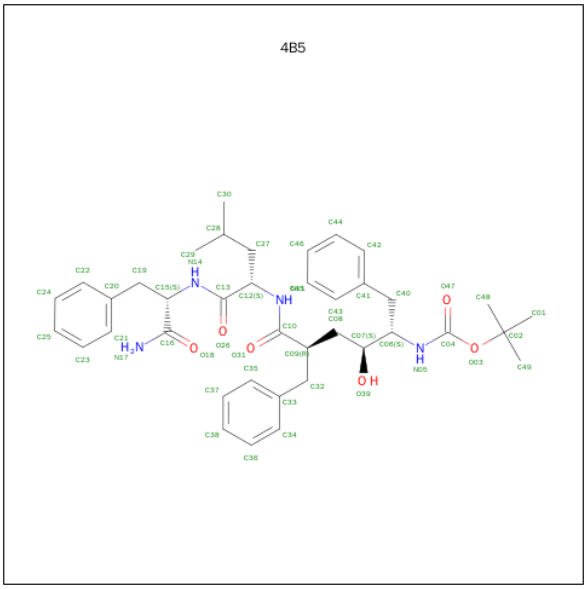
- Molecule 1 is a protein called Uncharacterized protein PSH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1802	1219	276	296	11			
1	B	245	Total	C	N	O	S	0	0	0
			1797	1217	275	294	11			
1	C	238	Total	C	N	O	S	0	0	0
			1763	1197	267	288	11			
1	D	237	Total	C	N	O	S	0	0	0
			1740	1180	264	285	11			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	ASN	ASP	engineered mutation	UNP A3CWV0
A	42	SER	GLU	engineered mutation	UNP A3CWV0
A	147	GLU	ALA	engineered mutation	UNP A3CWV0
A	148	PRO	VAL	engineered mutation	UNP A3CWV0
A	229	VAL	ALA	engineered mutation	UNP A3CWV0
B	40	ASN	ASP	engineered mutation	UNP A3CWV0
B	42	SER	GLU	engineered mutation	UNP A3CWV0
B	147	GLU	ALA	engineered mutation	UNP A3CWV0
B	148	PRO	VAL	engineered mutation	UNP A3CWV0
B	229	VAL	ALA	engineered mutation	UNP A3CWV0
C	40	ASN	ASP	engineered mutation	UNP A3CWV0
C	42	SER	GLU	engineered mutation	UNP A3CWV0
C	147	GLU	ALA	engineered mutation	UNP A3CWV0
C	148	PRO	VAL	engineered mutation	UNP A3CWV0
C	229	VAL	ALA	engineered mutation	UNP A3CWV0
D	40	ASN	ASP	engineered mutation	UNP A3CWV0
D	42	SER	GLU	engineered mutation	UNP A3CWV0
D	147	GLU	ALA	engineered mutation	UNP A3CWV0
D	148	PRO	VAL	engineered mutation	UNP A3CWV0
D	229	VAL	ALA	engineered mutation	UNP A3CWV0

- Molecule 2 is N-{(2R,4S,5S)-2-benzyl-5-[(tert-butoxycarbonyl)amino]-4-hydroxy-6-phenylhexanoyl}-L-leucyl-L-phenylalaninamide (three-letter code: 4B5) (formula: $C_{39}H_{52}N_4O_6$).



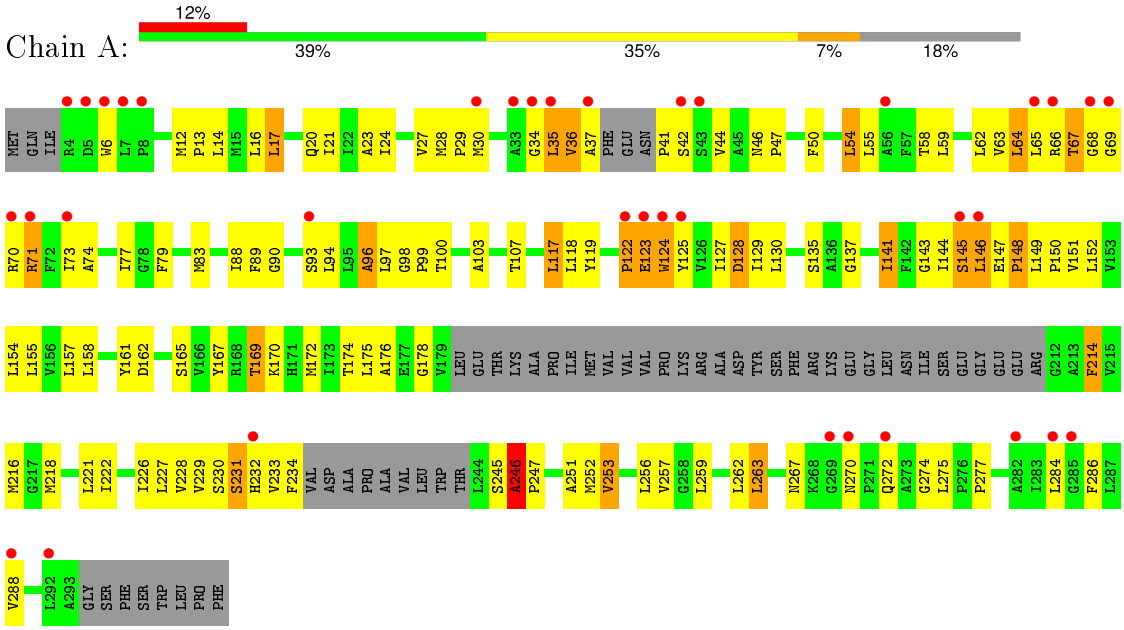
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			49	39	4	6		
2	D	1	Total	C	N	O	0	0
			49	39	4	6		

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 errors 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.

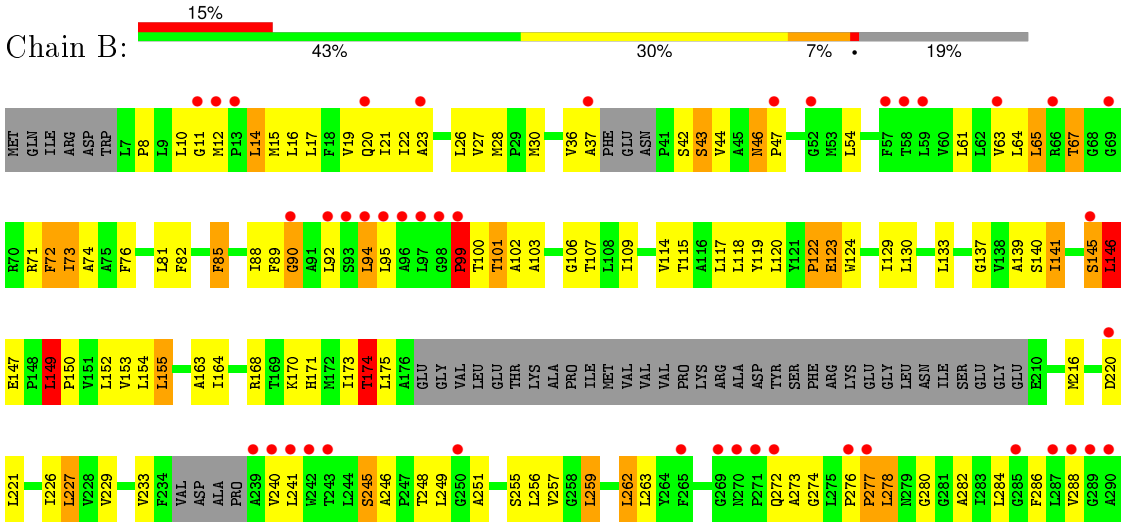
- Molecule 1: Uncharacterized protein PSH

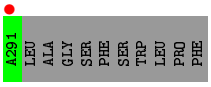
Chain A:



- Molecule 1: Uncharacterized protein PSH

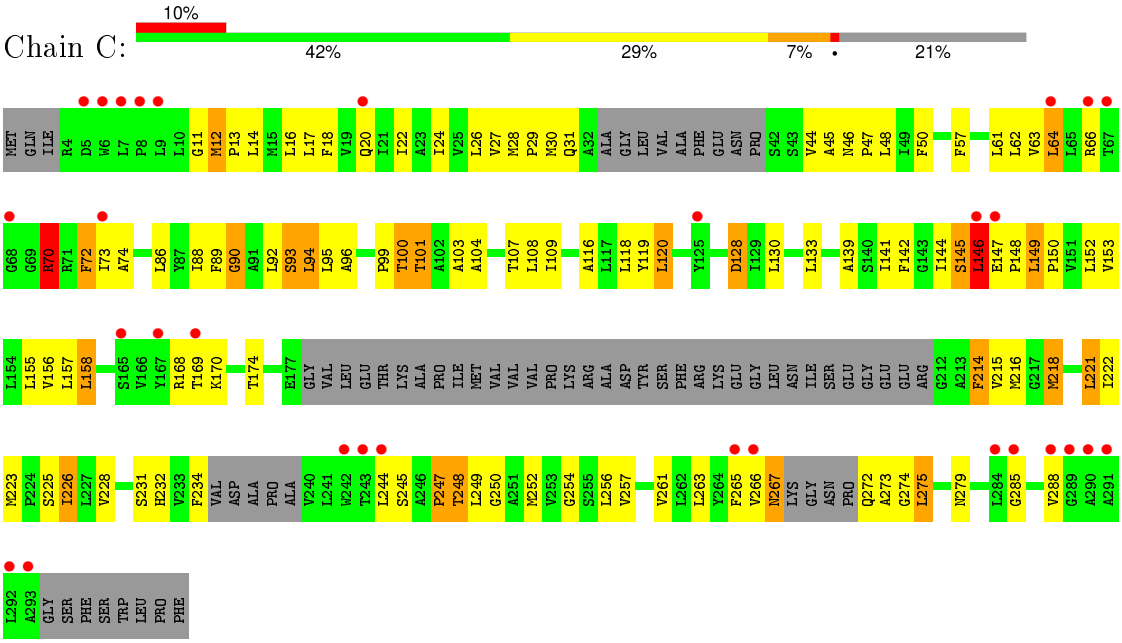
Chain B:





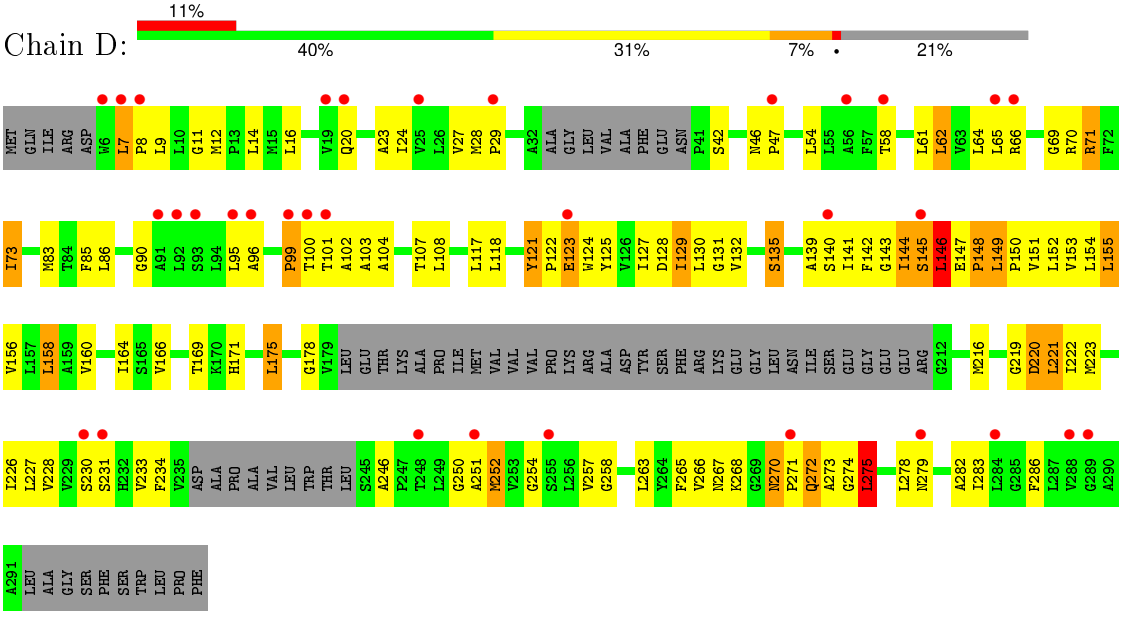
• Molecule 1: Uncharacterized protein PSH

Chain C:



• Molecule 1: Uncharacterized protein PSH

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	168.62Å 201.69Å 117.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.20 – 3.85 48.20 – 3.85	Depositor EDS
% Data completeness (in resolution range)	40.0 (48.20-3.85) 40.1 (48.20-3.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 3.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.320 , 0.367 0.332 , 0.362	Depositor DCC
R_{free} test set	361 reflections (4.90%)	DCC
Wilson B-factor (Å^2)	-6.1	Xtriage
Anisotropy	3.478	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 146.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 7735 reflections	Xtriage
F_o,F_c correlation	0.77	EDS
Total number of atoms	7200	wwPDB-VP
Average B, all atoms (Å^2)	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 4B5

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	0.29	0/1839	0.61	0/2511
1	B	0.31	0/1834	0.66	1/2505 (0.0%)
1	C	0.32	0/1799	0.70	2/2457 (0.1%)
1	D	0.34	0/1777	0.70	1/2427 (0.0%)
All	All	0.32	0/7249	0.67	4/9900 (0.0%)

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	A	0	5
1	B	0	3
1	C	0	2
1	D	0	1
All	All	0	11

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	275	LEU	CB-CG-CD1	6.28	121.67	111.00
1	C	275	LEU	CA-CB-CG	-6.01	101.49	115.30
1	C	146	LEU	CB-CG-CD2	5.58	120.49	111.00
1	B	278	LEU	CA-CB-CG	5.43	127.80	115.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	TRP	Peptide
1	A	145	SER	Peptide
1	A	146	LEU	Peptide
1	A	246	ALA	Peptide
1	A	272	GLN	Peptide
1	B	145	SER	Peptide
1	B	146	LEU	Peptide
1	B	99	PRO	Peptide
1	C	145	SER	Peptide
1	C	146	LEU	Peptide
1	D	146	LEU	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	A	1802	0	1949	65	0
1	B	1797	0	1949	68	0
1	C	1763	0	1903	74	0
1	D	1740	0	1881	93	0
2	C	49	0	52	13	0
2	D	49	0	52	9	0
All	All	7200	0	7786	296	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 20.

All (296) 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:265:PHE:HB3	1:D:271:PRO:HG2	1.47	0.94
1:D:139:ALA:HA	1:D:226:ILE:HG12	1.55	0.89
1:B:246:ALA:HA	1:B:249:LEU:HD12	1.55	0.88
1:D:216:MET:HE3	2:D:501:4B5:H34	1.58	0.85
1:D:151:VAL:HG13	1:D:227:LEU:HD13	1.56	0.85
1:D:251:ALA:HB2	1:D:286:PHE:HB2	1.59	0.84
1:C:100:THR:OG1	1:C:101:THR:N	2.04	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:MET:HE2	1:A:144:ILE:HD12	1.65	0.79
1:D:263:LEU:O	1:D:267:ASN:ND2	2.15	0.79
1:B:61:LEU:HA	1:B:64:LEU:HD12	1.65	0.78
1:A:36:VAL:HG12	1:A:37:ALA:H	1.47	0.78
1:A:253:VAL:HA	1:A:256:LEU:HD12	1.66	0.76
1:D:270:ASN:H	1:D:270:ASN:ND2	1.83	0.76
1:C:170:LYS:NZ	1:C:272:GLN:OE1	2.19	0.75
1:C:263:LEU:O	1:C:267:ASN:ND2	2.21	0.74
1:A:118:LEU:HD12	1:A:130:LEU:HD12	1.69	0.73
1:D:29:PRO:HB3	1:D:95:LEU:HG	1.69	0.73
1:D:129:ILE:HD13	1:D:130:LEU:HD23	1.70	0.73
1:B:100:THR:OG1	1:B:101:THR:N	2.21	0.73
1:D:147:GLU:HB3	1:D:148:PRO:HD2	1.72	0.72
1:B:36:VAL:HG12	1:B:37:ALA:H	1.55	0.71
1:C:26:LEU:HD22	1:C:92:LEU:HD13	1.72	0.71
1:C:169:THR:HG22	1:D:71:ARG:HH12	1.56	0.70
1:C:61:LEU:HD22	2:C:501:4B5:C45	2.22	0.70
1:D:155:LEU:HG	1:D:227:LEU:HD12	1.74	0.69
1:B:259:LEU:HB2	1:B:278:LEU:HD11	1.73	0.69
1:D:220:ASP:HB2	1:D:275:LEU:HD22	1.75	0.68
1:C:273:ALA:HB3	1:C:274:GLY:HA2	1.76	0.68
1:D:131:GLY:O	1:D:135:SER:OG	2.10	0.68
1:C:90:GLY:O	1:C:94:LEU:N	2.20	0.68
1:A:65:LEU:HD23	1:A:73:ILE:HD13	1.77	0.67
1:C:16:LEU:HA	1:C:221:LEU:HD11	1.77	0.67
1:D:216:MET:HE2	2:D:501:4B5:H25	1.60	0.66
1:B:65:LEU:HG	1:B:73:ILE:HD13	1.78	0.66
1:C:90:GLY:HA2	1:C:107:THR:HG21	1.79	0.65
1:B:262:LEU:HD23	1:B:263:LEU:HD23	1.77	0.65
1:D:143:GLY:HA2	1:D:230:SER:HB2	1.79	0.65
1:D:148:PRO:O	1:D:151:VAL:N	2.30	0.65
1:A:148:PRO:O	1:A:151:VAL:N	2.30	0.64
1:C:279:ASN:OD1	2:C:501:4B5:H29	1.97	0.64
1:A:63:VAL:O	1:A:67:THR:OG1	2.11	0.63
1:C:74:ALA:O	1:C:119:TYR:OH	2.09	0.63
1:B:73:ILE:HA	1:B:76:PHE:HB3	1.81	0.63
1:D:151:VAL:HG22	1:D:227:LEU:HD22	1.81	0.62
1:C:88:ILE:O	1:C:92:LEU:HB2	1.99	0.62
1:B:63:VAL:O	1:B:67:THR:OG1	2.11	0.62
1:C:103:ALA:O	1:C:107:THR:HG23	1.98	0.62
1:B:280:GLY:O	1:B:284:LEU:HG	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ALA:O	1:A:119:TYR:OH	2.17	0.61
1:D:24:ILE:O	1:D:27:VAL:HB	2.00	0.61
1:D:65:LEU:O	1:D:69:GLY:N	2.34	0.61
1:C:88:ILE:HA	1:C:92:LEU:HD12	1.83	0.61
1:D:146:LEU:O	1:D:230:SER:OG	2.17	0.60
1:D:61:LEU:HA	1:D:64:LEU:HD12	1.84	0.60
1:B:82:PHE:HA	1:B:115:THR:HG21	1.83	0.60
1:D:275:LEU:HB3	1:D:278:LEU:HB2	1.84	0.60
1:C:139:ALA:HA	1:C:226:ILE:HG13	1.84	0.60
1:B:171:HIS:HA	1:B:174:THR:HG23	1.85	0.59
1:B:251:ALA:HB2	1:B:286:PHE:HB2	1.83	0.59
1:B:85:PHE:HE1	1:B:133:LEU:HD23	1.66	0.59
1:B:146:LEU:HD12	1:B:147:GLU:HG2	1.83	0.59
1:C:158:LEU:HD12	2:C:501:4B5:H22	1.85	0.59
1:A:36:VAL:HG13	1:A:145:SER:HA	1.85	0.58
1:A:98:GLY:O	1:A:100:THR:N	2.36	0.58
1:D:216:MET:CE	2:D:501:4B5:H34	2.32	0.58
1:D:145:SER:O	1:D:146:LEU:HD13	2.04	0.58
1:C:275:LEU:HD13	2:C:501:4B5:C22	2.33	0.58
1:D:254:GLY:HA2	1:D:257:VAL:HG12	1.84	0.58
1:D:258:GLY:HA3	1:D:278:LEU:HD13	1.85	0.58
1:D:275:LEU:HA	1:D:278:LEU:HD23	1.85	0.58
1:C:247:PRO:O	1:C:250:GLY:N	2.35	0.57
1:A:263:LEU:O	1:A:267:ASN:ND2	2.33	0.57
1:D:148:PRO:HD3	1:D:230:SER:O	2.05	0.57
1:D:54:LEU:O	1:D:58:THR:HG23	2.04	0.57
1:D:100:THR:HG21	1:D:104:ALA:HB2	1.87	0.57
1:B:74:ALA:O	1:B:119:TYR:OH	2.23	0.57
1:A:147:GLU:HB3	1:A:148:PRO:HD2	1.86	0.56
1:C:118:LEU:HD12	1:C:130:LEU:HD12	1.87	0.56
1:B:88:ILE:HD11	1:B:137:GLY:HA3	1.88	0.56
1:A:262:LEU:HD23	1:A:277:PRO:HG2	1.88	0.56
1:B:155:LEU:HD12	1:B:227:LEU:HD12	1.86	0.56
1:A:17:LEU:HD21	1:A:256:LEU:HD11	1.88	0.56
1:A:165:SER:O	1:A:169:THR:HG23	2.07	0.55
1:D:155:LEU:HD22	1:D:279:ASN:ND2	2.22	0.55
1:B:22:ILE:O	1:B:26:LEU:HG	2.06	0.55
1:A:30:MET:HE1	1:A:141:ILE:HA	1.88	0.55
1:C:222:ILE:O	1:C:225:SER:OG	2.19	0.55
1:A:167:TYR:HD2	1:B:120:LEU:HD22	1.70	0.55
1:C:45:ALA:HA	1:C:48:LEU:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:VAL:O	1:D:164:ILE:HG12	2.08	0.54
1:C:57:PHE:HE2	2:C:501:4B5:H44	1.73	0.54
1:D:70:ARG:O	1:D:71:ARG:HB2	2.08	0.54
1:A:246:ALA:HB1	1:A:247:PRO:HD2	1.90	0.54
1:C:11:GLY:O	1:C:14:LEU:HB3	2.08	0.54
1:C:257:VAL:O	1:C:261:VAL:HG23	2.08	0.53
1:D:155:LEU:HD12	1:D:283:ILE:HG13	1.90	0.53
1:D:151:VAL:HG13	1:D:227:LEU:HB3	1.91	0.53
1:D:250:GLY:O	1:D:254:GLY:N	2.38	0.53
1:D:16:LEU:O	1:D:20:GLN:HG3	2.07	0.53
1:A:41:PRO:C	1:A:146:LEU:HG	2.29	0.53
1:A:218:MET:O	1:A:221:LEU:HB3	2.08	0.53
1:A:229:VAL:O	1:A:231:SER:N	2.42	0.52
1:C:158:LEU:HD12	2:C:501:4B5:C19	2.39	0.52
1:A:228:VAL:HG21	1:A:252:MET:HG3	1.91	0.52
1:B:173:ILE:O	1:B:175:LEU:N	2.42	0.52
1:A:90:GLY:HA2	1:A:107:THR:HG21	1.90	0.52
1:D:219:GLY:O	1:D:222:ILE:HB	2.09	0.52
1:A:24:ILE:HA	1:A:27:VAL:HG23	1.91	0.52
1:B:16:LEU:O	1:B:20:GLN:HG3	2.10	0.52
1:D:272:GLN:HE22	1:D:275:LEU:H	1.57	0.52
1:B:90:GLY:O	1:B:94:LEU:HB3	2.09	0.52
1:B:94:LEU:HD11	1:B:100:THR:HA	1.91	0.52
1:C:275:LEU:HD13	2:C:501:4B5:C24	2.40	0.52
1:D:7:LEU:HB2	1:D:8:PRO:HD3	1.91	0.52
1:B:241:LEU:HA	1:B:245:SER:H	1.75	0.52
1:A:54:LEU:O	1:A:58:THR:HG23	2.08	0.52
1:D:139:ALA:HA	1:D:226:ILE:CG1	2.35	0.52
1:C:222:ILE:HG22	1:C:226:ILE:HD12	1.92	0.51
1:D:125:TYR:O	1:D:129:ILE:HG22	2.11	0.51
1:D:227:LEU:HA	1:D:230:SER:HB3	1.93	0.51
1:A:170:LYS:O	1:A:174:THR:HG23	2.11	0.51
1:C:44:VAL:HA	1:C:150:PRO:HG3	1.91	0.51
1:A:42:SER:HB2	1:A:146:LEU:HD12	1.92	0.51
1:D:142:PHE:HB2	1:D:226:ILE:HD13	1.91	0.51
1:D:16:LEU:HA	1:D:221:LEU:HD11	1.93	0.51
1:D:154:LEU:HD23	1:D:227:LEU:HD11	1.92	0.51
1:B:47:PRO:HB3	1:B:154:LEU:HB2	1.92	0.50
1:D:11:GLY:O	1:D:14:LEU:HB3	2.12	0.50
1:B:26:LEU:HD22	1:B:92:LEU:HB3	1.93	0.50
1:B:19:VAL:HG21	1:B:221:LEU:HG	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:HD23	1:B:72:PHE:CZ	2.46	0.50
1:B:43:SER:O	1:B:46:ASN:HB2	2.11	0.50
1:A:251:ALA:HB2	1:A:286:PHE:HB2	1.93	0.50
1:C:247:PRO:O	1:C:249:LEU:N	2.45	0.49
1:C:16:LEU:O	1:C:20:GLN:HG3	2.11	0.49
1:D:118:LEU:HD12	1:D:130:LEU:HD12	1.95	0.49
1:C:94:LEU:HD11	1:C:104:ALA:HA	1.93	0.49
1:B:30:MET:HE1	1:B:141:ILE:HA	1.94	0.49
1:D:149:LEU:HB3	1:D:150:PRO:HD3	1.94	0.49
1:C:20:GLN:NE2	1:C:252:MET:HG2	2.27	0.49
1:A:24:ILE:O	1:A:27:VAL:N	2.45	0.49
1:B:102:ALA:O	1:B:106:GLY:N	2.41	0.49
1:A:23:ALA:O	1:A:27:VAL:HG23	2.12	0.49
1:C:216:MET:SD	2:C:501:4B5:H34	2.53	0.49
1:D:28:MET:HB3	1:D:29:PRO:HD3	1.94	0.49
1:C:223:MET:HG3	2:C:501:4B5:C24	2.43	0.49
1:D:83:MET:O	1:D:86:LEU:HB2	2.12	0.49
1:C:12:MET:SD	1:C:13:PRO:HD3	2.52	0.49
1:B:100:THR:HG1	1:B:101:THR:H	1.58	0.49
1:D:62:LEU:HD12	1:D:65:LEU:HD12	1.95	0.49
1:C:29:PRO:HG2	1:C:92:LEU:HD22	1.94	0.49
1:C:12:MET:N	1:C:13:PRO:HD2	2.27	0.49
1:B:30:MET:HG2	1:B:92:LEU:HD21	1.94	0.48
1:C:47:PRO:O	1:C:50:PHE:HB3	2.13	0.48
1:D:65:LEU:HG	1:D:73:ILE:HD12	1.94	0.48
1:A:16:LEU:HA	1:A:221:LEU:HD11	1.94	0.48
1:D:42:SER:H	1:D:146:LEU:HD11	1.78	0.48
1:B:94:LEU:O	1:B:99:PRO:HA	2.12	0.48
2:D:501:4B5:H16	2:D:501:4B5:H34	1.94	0.48
1:B:89:PHE:HB3	1:B:107:THR:HB	1.95	0.48
1:D:270:ASN:N	1:D:270:ASN:ND2	2.59	0.48
1:C:169:THR:HG22	1:D:71:ARG:NH1	2.27	0.47
1:C:16:LEU:HD23	1:C:256:LEU:HD23	1.96	0.47
1:D:228:VAL:HG22	1:D:251:ALA:HB1	1.97	0.47
1:A:13:PRO:HD3	1:A:259:LEU:HD21	1.96	0.47
1:C:231:SER:HB3	1:C:248:THR:HG22	1.96	0.47
1:B:16:LEU:HD23	1:B:256:LEU:HD23	1.95	0.47
1:B:103:ALA:O	1:B:107:THR:HG23	2.14	0.47
1:B:255:SER:HB2	1:B:282:ALA:HB2	1.97	0.47
1:B:23:ALA:O	1:B:27:VAL:HG23	2.15	0.47
1:C:254:GLY:HA3	1:C:285:GLY:HA3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:TRP:HA	1:A:127:ILE:HG12	1.97	0.46
1:C:72:PHE:HD1	1:C:72:PHE:H	1.62	0.46
2:D:501:4B5:H41	2:D:501:4B5:H15	1.69	0.46
1:D:216:MET:HE2	2:D:501:4B5:N11	2.27	0.46
1:A:149:LEU:HB3	1:A:150:PRO:HD3	1.97	0.46
1:C:275:LEU:HB3	2:C:501:4B5:C23	2.46	0.46
1:C:149:LEU:HB3	1:C:150:PRO:HD3	1.98	0.46
1:D:158:LEU:HA	1:D:158:LEU:HD23	1.72	0.46
1:A:262:LEU:HD21	1:A:274:GLY:HA2	1.97	0.46
1:B:149:LEU:HB3	1:B:150:PRO:HD3	1.96	0.46
1:B:140:SER:HA	1:B:229:VAL:HG21	1.98	0.46
1:A:28:MET:HB3	1:A:29:PRO:HD3	1.97	0.46
1:D:273:ALA:HA	1:D:274:GLY:HA2	1.57	0.46
1:D:100:THR:HB	1:D:103:ALA:HB3	1.98	0.46
1:D:90:GLY:HA2	1:D:107:THR:HG21	1.97	0.46
1:C:116:ALA:O	1:C:120:LEU:HG	2.16	0.46
1:A:58:THR:O	1:A:62:LEU:HG	2.16	0.46
1:D:158:LEU:HD13	2:D:501:4B5:H23	1.97	0.45
1:D:166:VAL:HG21	1:D:273:ALA:N	2.32	0.45
1:C:214:PHE:O	1:C:218:MET:HG3	2.16	0.45
1:D:103:ALA:O	1:D:107:THR:HG23	2.17	0.45
1:A:135:SER:HA	1:A:222:ILE:HD11	1.98	0.45
1:A:93:SER:HA	1:A:96:ALA:HB3	1.98	0.45
1:B:118:LEU:HD12	1:B:130:LEU:HD12	1.98	0.45
1:C:24:ILE:O	1:C:27:VAL:HG12	2.17	0.45
1:D:227:LEU:N	1:D:227:LEU:HD23	2.31	0.45
1:A:94:LEU:O	1:A:98:GLY:HA2	2.16	0.45
1:B:17:LEU:HG	1:B:256:LEU:HD21	1.99	0.45
1:C:24:ILE:HD11	1:C:228:VAL:HG12	1.98	0.45
2:D:501:4B5:H16	2:D:501:4B5:C34	2.47	0.45
1:B:163:ALA:HB2	1:B:276:PRO:CG	2.46	0.45
1:D:47:PRO:HB3	1:D:154:LEU:HB2	1.98	0.45
1:A:68:GLY:HA2	1:A:69:GLY:HA3	1.62	0.45
1:D:101:THR:OG1	1:D:102:ALA:N	2.50	0.45
1:B:129:ILE:HG22	1:B:130:LEU:HD23	1.98	0.44
1:A:27:VAL:HA	1:A:144:ILE:HD11	2.00	0.44
1:C:93:SER:HA	1:C:96:ALA:HB3	1.98	0.44
1:D:254:GLY:HA3	1:D:282:ALA:HA	1.99	0.44
1:A:103:ALA:O	1:A:107:THR:HG23	2.17	0.44
1:D:27:VAL:O	1:D:144:ILE:HD11	2.16	0.44
1:D:171:HIS:CE1	1:D:175:LEU:HD13	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:LEU:O	1:B:64:LEU:HB2	2.18	0.44
1:C:275:LEU:HD12	2:C:501:4B5:H12	2.00	0.44
1:B:88:ILE:O	1:B:92:LEU:HB2	2.18	0.44
1:A:88:ILE:HD11	1:A:137:GLY:HA3	1.99	0.44
1:D:272:GLN:NE2	1:D:275:LEU:H	2.16	0.44
1:C:275:LEU:HD23	1:C:275:LEU:HA	1.68	0.44
1:C:99:PRO:HB2	1:C:100:THR:HG22	1.99	0.44
1:B:85:PHE:CE1	1:B:133:LEU:HD23	2.49	0.44
1:A:128:ASP:N	1:A:128:ASP:OD1	2.51	0.44
1:A:47:PRO:HB3	1:A:154:LEU:HB2	1.98	0.44
1:D:155:LEU:CG	1:D:227:LEU:HD12	2.45	0.44
1:A:36:VAL:HG12	1:A:37:ALA:N	2.24	0.44
1:A:161:TYR:HE2	1:B:71:ARG:HH21	1.66	0.44
1:B:173:ILE:C	1:B:175:LEU:H	2.21	0.43
1:B:149:LEU:HD22	1:B:149:LEU:HA	1.87	0.43
1:C:86:LEU:HA	1:C:86:LEU:HD23	1.88	0.43
1:B:47:PRO:HG3	1:B:150:PRO:O	2.17	0.43
1:C:28:MET:HB3	1:C:29:PRO:HD3	1.99	0.43
1:B:146:LEU:HA	1:B:146:LEU:HD13	1.76	0.43
1:D:23:ALA:O	1:D:27:VAL:HG23	2.18	0.43
1:D:20:GLN:OE1	1:D:252:MET:HG2	2.17	0.43
1:B:122:PRO:HB2	1:B:123:GLU:H	1.52	0.43
1:B:164:ILE:O	1:B:168:ARG:HB2	2.19	0.43
1:D:275:LEU:CB	1:D:278:LEU:HB2	2.47	0.43
1:D:99:PRO:HA	1:D:100:THR:HA	1.77	0.43
1:A:127:ILE:HG22	1:A:214:PHE:HE2	1.83	0.43
1:A:123:GLU:HB3	1:A:125:TYR:CE2	2.53	0.43
1:D:24:ILE:O	1:D:27:VAL:N	2.50	0.43
1:D:128:ASP:O	1:D:132:VAL:HG23	2.19	0.43
1:D:272:GLN:H	1:D:273:ALA:HA	1.84	0.43
1:D:123:GLU:O	1:D:125:TYR:N	2.51	0.43
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.83	0.43
1:A:20:GLN:OE1	1:A:252:MET:HG2	2.17	0.43
1:B:11:GLY:O	1:B:14:LEU:HB3	2.19	0.43
1:A:20:GLN:CD	1:A:252:MET:HG2	2.40	0.42
1:C:29:PRO:HG2	1:C:92:LEU:CD2	2.49	0.42
1:C:215:VAL:HG11	2:C:501:4B5:C45	2.49	0.42
1:C:64:LEU:HD21	1:C:73:ILE:HA	2.01	0.42
1:D:151:VAL:CG2	1:D:227:LEU:HD22	2.47	0.42
1:C:86:LEU:O	1:C:90:GLY:N	2.52	0.42
1:C:218:MET:O	1:C:222:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:VAL:O	1:C:144:ILE:HD11	2.20	0.42
1:C:148:PRO:HG2	1:C:234:PHE:HD2	1.84	0.42
1:D:226:ILE:HG22	1:D:227:LEU:HD23	2.02	0.42
1:A:143:GLY:HA3	1:A:229:VAL:HB	2.01	0.42
1:D:223:MET:HG3	2:D:501:4B5:C22	2.49	0.42
1:C:72:PHE:CD1	1:C:72:PHE:N	2.88	0.42
1:A:117:LEU:HD22	1:A:122:PRO:HB3	2.02	0.42
1:C:146:LEU:HD12	1:C:147:GLU:CD	2.40	0.42
1:C:28:MET:O	1:C:31:GLN:HG2	2.19	0.42
1:A:97:LEU:HB2	1:A:103:ALA:HB2	2.01	0.42
1:B:139:ALA:HA	1:B:226:ILE:CD1	2.49	0.42
1:B:119:TYR:O	1:B:120:LEU:HB2	2.19	0.42
1:B:26:LEU:HD22	1:B:92:LEU:HD13	2.02	0.42
1:C:70:ARG:HD3	1:C:70:ARG:HA	1.62	0.42
1:A:162:ASP:HB2	1:A:275:LEU:HD12	2.02	0.42
1:D:274:GLY:O	1:D:275:LEU:HB2	2.19	0.41
1:A:64:LEU:HD11	1:A:73:ILE:HG23	2.02	0.41
1:D:151:VAL:CG1	1:D:227:LEU:HB3	2.50	0.41
1:B:145:SER:O	1:B:146:LEU:HB2	2.20	0.41
1:C:249:LEU:HA	1:C:252:MET:HE2	2.02	0.41
1:D:227:LEU:O	1:D:231:SER:HB3	2.21	0.41
1:B:233:VAL:O	1:B:233:VAL:HG12	2.20	0.41
1:D:271:PRO:HA	1:D:272:GLN:HA	1.77	0.41
1:A:59:LEU:HB2	1:B:72:PHE:CE1	2.56	0.41
1:B:8:PRO:O	1:B:11:GLY:N	2.54	0.41
1:A:36:VAL:CG1	1:A:37:ALA:H	2.26	0.41
1:A:71:ARG:HB2	1:A:71:ARG:NH1	2.35	0.41
1:D:140:SER:O	1:D:144:ILE:HB	2.20	0.41
1:A:34:GLY:O	1:A:35:LEU:HB2	2.20	0.41
1:B:276:PRO:N	1:B:277:PRO:HD2	2.35	0.41
1:C:128:ASP:OD1	1:C:128:ASP:N	2.54	0.41
1:A:146:LEU:HA	1:A:146:LEU:HD13	1.84	0.41
1:B:114:VAL:HG13	1:B:130:LEU:HD13	2.03	0.41
1:C:18:PHE:O	1:C:22:ILE:HG13	2.21	0.41
1:C:157:LEU:HD11	1:D:108:LEU:HD21	2.03	0.40
1:D:121:TYR:HA	1:D:122:PRO:HD2	1.80	0.40
1:A:98:GLY:C	1:A:100:THR:H	2.23	0.40
1:D:151:VAL:HG13	1:D:227:LEU:CD1	2.38	0.40
1:A:89:PHE:HB3	1:A:107:THR:HB	2.03	0.40
1:C:142:PHE:HA	1:C:145:SER:HB3	2.03	0.40
1:C:216:MET:CE	2:C:501:4B5:H26	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:LEU:HD21	1:C:108:LEU:HA	2.03	0.40
1:B:21:ILE:HG22	1:B:22:ILE:HD13	2.04	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	238/301 (79%)	198 (83%)	27 (11%)	13 (6%)	2 29
1	B	237/301 (79%)	198 (84%)	23 (10%)	16 (7%)	1 23
1	C	228/301 (76%)	192 (84%)	25 (11%)	11 (5%)	3 32
1	D	229/301 (76%)	192 (84%)	23 (10%)	14 (6%)	2 26
All	All	932/1204 (77%)	780 (84%)	98 (10%)	54 (6%)	2 27

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	99	PRO
1	A	122	PRO
1	A	246	ALA
1	B	42	SER
1	B	43	SER
1	B	72	PHE
1	B	99	PRO
1	B	149	LEU
1	C	120	LEU
1	C	248	THR
1	D	71	ARG
1	D	124	TRP

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Mol	Chain	Res	Type
1	D	148	PRO
1	D	275	LEU
1	A	35	LEU
1	A	96	ALA
1	A	230	SER
1	A	231	SER
1	B	101	THR
1	B	122	PRO
1	B	123	GLU
1	B	124	TRP
1	B	146	LEU
1	B	174	THR
1	B	274	GLY
1	C	89	PHE
1	C	93	SER
1	C	146	LEU
1	C	245	SER
1	D	96	ALA
1	D	178	GLY
1	D	268	LYS
1	A	148	PRO
1	A	178	GLY
1	B	277	PRO
1	D	7	LEU
1	D	99	PRO
1	D	123	GLU
1	A	6	TRP
1	B	90	GLY
1	B	240	VAL
1	C	70	ARG
1	C	101	THR
1	C	244	LEU
1	D	121	TYR
1	D	234	PHE
1	B	273	ALA
1	A	176	ALA
1	C	90	GLY
1	D	246	ALA
1	D	233	VAL
1	A	270	ASN
1	C	247	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	188/236 (80%)	146 (78%)	42 (22%)	1 9
1	B	188/236 (80%)	153 (81%)	35 (19%)	2 15
1	C	185/236 (78%)	151 (82%)	34 (18%)	2 15
1	D	183/236 (78%)	154 (84%)	29 (16%)	3 23
All	All	744/944 (79%)	604 (81%)	140 (19%)	2 15

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

Mol	Chain	Res	Type
1	A	12	MET
1	A	14	LEU
1	A	17	LEU
1	A	21	ILE
1	A	44	VAL
1	A	46	ASN
1	A	50	PHE
1	A	54	LEU
1	A	55	LEU
1	A	64	LEU
1	A	66	ARG
1	A	67	THR
1	A	70	ARG
1	A	71	ARG
1	A	77	ILE
1	A	79	PHE
1	A	83	MET
1	A	117	LEU
1	A	123	GLU
1	A	128	ASP
1	A	129	ILE
1	A	141	ILE
1	A	152	LEU
1	A	155	LEU

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Mol	Chain	Res	Type
1	A	157	LEU
1	A	158	LEU
1	A	169	THR
1	A	172	MET
1	A	175	LEU
1	A	214	PHE
1	A	216	MET
1	A	226	ILE
1	A	227	LEU
1	A	232	HIS
1	A	233	VAL
1	A	234	PHE
1	A	245	SER
1	A	253	VAL
1	A	257	VAL
1	A	263	LEU
1	A	284	LEU
1	A	288	VAL
1	B	10	LEU
1	B	12	MET
1	B	14	LEU
1	B	15	MET
1	B	28	MET
1	B	44	VAL
1	B	46	ASN
1	B	54	LEU
1	B	65	LEU
1	B	67	THR
1	B	73	ILE
1	B	81	LEU
1	B	85	PHE
1	B	94	LEU
1	B	95	LEU
1	B	109	ILE
1	B	117	LEU
1	B	141	ILE
1	B	146	LEU
1	B	149	LEU
1	B	152	LEU
1	B	153	VAL
1	B	155	LEU
1	B	170	LYS

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Mol	Chain	Res	Type
1	B	174	THR
1	B	216	MET
1	B	220	ASP
1	B	227	LEU
1	B	245	SER
1	B	248	THR
1	B	257	VAL
1	B	259	LEU
1	B	262	LEU
1	B	272	GLN
1	B	288	VAL
1	C	12	MET
1	C	17	LEU
1	C	30	MET
1	C	46	ASN
1	C	62	LEU
1	C	63	VAL
1	C	64	LEU
1	C	66	ARG
1	C	70	ARG
1	C	72	PHE
1	C	94	LEU
1	C	95	LEU
1	C	100	THR
1	C	109	ILE
1	C	128	ASP
1	C	133	LEU
1	C	141	ILE
1	C	149	LEU
1	C	152	LEU
1	C	153	VAL
1	C	155	LEU
1	C	156	VAL
1	C	158	LEU
1	C	168	ARG
1	C	174	THR
1	C	214	PHE
1	C	218	MET
1	C	221	LEU
1	C	226	ILE
1	C	232	HIS
1	C	265	PHE

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Mol	Chain	Res	Type
1	C	266	VAL
1	C	267	ASN
1	C	288	VAL
1	D	9	LEU
1	D	12	MET
1	D	46	ASN
1	D	62	LEU
1	D	66	ARG
1	D	73	ILE
1	D	85	PHE
1	D	117	LEU
1	D	127	ILE
1	D	129	ILE
1	D	135	SER
1	D	141	ILE
1	D	144	ILE
1	D	145	SER
1	D	146	LEU
1	D	149	LEU
1	D	152	LEU
1	D	153	VAL
1	D	155	LEU
1	D	156	VAL
1	D	158	LEU
1	D	169	THR
1	D	175	LEU
1	D	220	ASP
1	D	221	LEU
1	D	252	MET
1	D	266	VAL
1	D	270	ASN
1	D	272	GLN

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

Mol	Chain	Res	Type
1	C	20	GLN

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands 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	$\#\|Z\| > 2$
2	4B5	C	501	-	51,51,51	1.92	9 (17%)	64,69,69	1.35	7 (10%)
2	4B5	D	501	-	51,51,51	1.97	7 (13%)	64,69,69	1.50	10 (15%)

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
2	4B5	C	501	-	-	0/53/53/53	0/3/3/3
2	4B5	D	501	-	-	0/53/53/53	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	4B5	C15-C16	-2.01	1.49	1.52
2	C	501	4B5	O39-C07	-2.00	1.38	1.43
2	C	501	4B5	C40-C41	2.19	1.56	1.51
2	D	501	4B5	C40-C41	2.29	1.56	1.51
2	C	501	4B5	C32-C33	2.37	1.57	1.51
2	D	501	4B5	C32-C33	2.82	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	4B5	C04-N05	4.53	1.47	1.34
2	D	501	4B5	C04-N05	4.56	1.47	1.34
2	C	501	4B5	C16-N17	4.70	1.42	1.32
2	C	501	4B5	O03-C04	4.75	1.45	1.34
2	D	501	4B5	O03-C04	4.91	1.45	1.34
2	D	501	4B5	C16-N17	4.95	1.42	1.32
2	D	501	4B5	C10-N11	5.98	1.47	1.34
2	C	501	4B5	C10-N11	6.00	1.47	1.34
2	C	501	4B5	C13-N14	6.08	1.48	1.34
2	D	501	4B5	C13-N14	6.24	1.48	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	4B5	O47-C04-N05	-3.22	119.24	124.86
2	C	501	4B5	C02-O03-C04	-3.16	115.95	121.05
2	C	501	4B5	C28-C27-C12	-3.08	106.39	115.50
2	C	501	4B5	O47-C04-N05	-2.93	119.74	124.86
2	D	501	4B5	C28-C27-C12	-2.78	107.27	115.50
2	D	501	4B5	C02-O03-C04	-2.70	116.69	121.05
2	D	501	4B5	O03-C04-O47	-2.59	120.33	125.55
2	C	501	4B5	O03-C04-O47	-2.58	120.33	125.55
2	D	501	4B5	O31-C10-C09	-2.13	119.36	122.12
2	D	501	4B5	O18-C16-N17	-2.09	119.98	123.08
2	C	501	4B5	C15-C16-N17	2.24	120.22	116.60
2	C	501	4B5	C33-C32-C09	2.44	118.29	113.70
2	D	501	4B5	C15-C16-N17	2.58	120.77	116.60
2	D	501	4B5	C12-N11-C10	3.02	128.38	121.62
2	D	501	4B5	C33-C32-C09	5.03	123.16	113.70
2	C	501	4B5	O03-C04-N05	5.26	119.92	110.07
2	D	501	4B5	O03-C04-N05	5.53	120.43	110.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	4B5	13	0
2	D	501	4B5	9	0

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, 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	246/301 (81%)	0.78	36 (14%)	3 3	56, 135, 215, 283	0
1	B	245/301 (81%)	0.96	44 (17%)	2 2	72, 161, 226, 290	0
1	C	238/301 (79%)	0.71	30 (12%)	5 5	66, 150, 247, 304	0
1	D	237/301 (78%)	0.92	33 (13%)	4 4	64, 168, 248, 290	0
All	All	966/1204 (80%)	0.84	143 (14%)	3 3	56, 152, 239, 304	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	TRP	8.3
1	A	5	ASP	7.6
1	A	270	ASN	7.1
1	D	6	TRP	6.9
1	C	68	GLY	6.5
1	C	288	VAL	6.5
1	B	289	GLY	6.2
1	A	34	GLY	5.7
1	B	242	TRP	5.6
1	D	93	SER	5.5
1	C	8	PRO	5.4
1	B	94	LEU	5.4
1	B	92	LEU	5.3
1	B	93	SER	5.0
1	B	288	VAL	5.0
1	A	8	PRO	5.0
1	D	96	ALA	4.9
1	D	7	LEU	4.5
1	A	68	GLY	4.5
1	C	5	ASP	4.4
1	B	98	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	69	GLY	4.3
1	B	95	LEU	4.3
1	C	289	GLY	4.2
1	B	58	THR	3.9
1	C	242	TRP	3.8
1	D	91	ALA	3.8
1	B	99	PRO	3.7
1	A	69	GLY	3.5
1	B	239	ALA	3.5
1	A	65	LEU	3.5
1	D	58	THR	3.4
1	B	13	PRO	3.4
1	D	288	VAL	3.4
1	D	66	ARG	3.4
1	A	7	LEU	3.4
1	C	290	ALA	3.4
1	D	95	LEU	3.4
1	C	293	ALA	3.4
1	D	145	SER	3.4
1	B	271	PRO	3.3
1	D	251	ALA	3.3
1	D	8	PRO	3.3
1	B	96	ALA	3.2
1	C	67	THR	3.2
1	C	244	LEU	3.2
1	A	124	TRP	3.1
1	B	287	LEU	3.1
1	D	123	GLU	3.0
1	A	71	ARG	3.0
1	D	92	LEU	3.0
1	C	7	LEU	3.0
1	D	100	THR	3.0
1	A	292	LEU	2.9
1	C	284	LEU	2.9
1	B	240	VAL	2.8
1	C	66	ARG	2.8
1	D	279	ASN	2.8
1	B	269	GLY	2.8
1	B	290	ALA	2.8
1	D	101	THR	2.8
1	D	29	PRO	2.8
1	A	145	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	9	LEU	2.8
1	B	220	ASP	2.7
1	D	231	SER	2.7
1	D	284	LEU	2.7
1	C	167	TYR	2.7
1	D	140	SER	2.7
1	C	20	GLN	2.7
1	D	56	ALA	2.7
1	A	37	ALA	2.7
1	B	145	SER	2.7
1	A	33	ALA	2.6
1	B	277	PRO	2.5
1	B	265	PHE	2.5
1	C	243	THR	2.5
1	C	64	LEU	2.5
1	C	147	GLU	2.5
1	C	285	GLY	2.5
1	B	66	ARG	2.5
1	A	284	LEU	2.5
1	B	11	GLY	2.5
1	D	65	LEU	2.5
1	B	63	VAL	2.5
1	B	276	PRO	2.5
1	A	272	GLN	2.5
1	B	250	GLY	2.5
1	C	292	LEU	2.4
1	A	35	LEU	2.4
1	A	73	ILE	2.4
1	A	4	ARG	2.4
1	B	243	THR	2.4
1	A	66	ARG	2.4
1	C	6	TRP	2.4
1	D	248	THR	2.4
1	B	241	LEU	2.4
1	D	271	PRO	2.4
1	D	255	SER	2.4
1	B	37	ALA	2.3
1	C	125	TYR	2.3
1	B	270	ASN	2.3
1	D	47	PRO	2.3
1	A	282	ALA	2.3
1	D	20	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	146	LEU	2.3
1	A	56	ALA	2.3
1	B	12	MET	2.3
1	C	165	SER	2.2
1	D	19	VAL	2.2
1	A	30	MET	2.2
1	C	146	LEU	2.2
1	B	272	GLN	2.2
1	C	169	THR	2.2
1	A	43	SER	2.2
1	A	93	SER	2.2
1	B	57	PHE	2.2
1	C	73	ILE	2.2
1	A	70	ARG	2.2
1	B	285	GLY	2.2
1	A	288	VAL	2.2
1	D	99	PRO	2.2
1	B	59	LEU	2.1
1	C	266	VAL	2.1
1	B	23	ALA	2.1
1	A	269	GLY	2.1
1	D	230	SER	2.1
1	A	122	PRO	2.1
1	A	42	SER	2.1
1	A	123	GLU	2.1
1	B	47	PRO	2.1
1	A	125	TYR	2.1
1	C	265	PHE	2.1
1	B	20	GLN	2.1
1	A	285	GLY	2.0
1	B	52	GLY	2.0
1	B	97	LEU	2.0
1	A	232	HIS	2.0
1	B	90	GLY	2.0
1	D	25	VAL	2.0
1	C	291	ALA	2.0
1	D	289	GLY	2.0
1	B	291	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	4B5	C	501	49/49	0.84	0.43	1.26	0,105,124,124	0
2	4B5	D	501	49/49	0.91	0.27	-0.63	32,60,73,74	0

6.5 Other polymers (i)

There are no such residues in this entry.