Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:51 AM GMT

PDB ID	:	3G6J
Title	:	C3b in complex with a C3b specific Fab
Authors	:	Wiesmann, C.
Deposited on	:	2009-02-06
Resolution	:	3.10 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

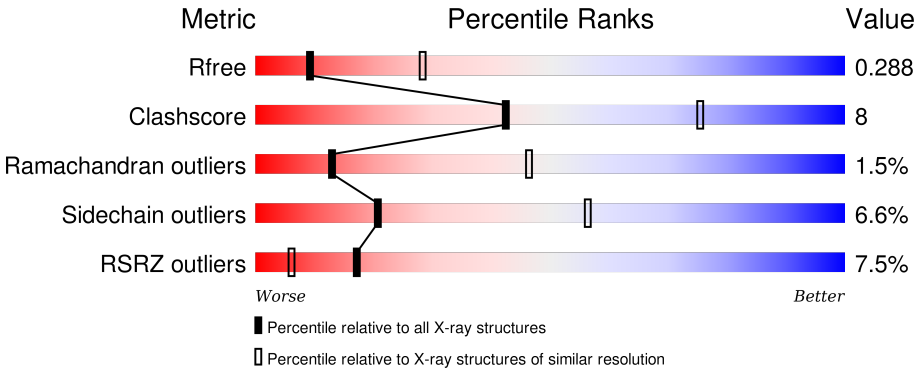
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	644	77%, 19%
1	C	644	79%, 19%
2	B	915	22%, 75%, 22%
2	D	915	9%, 77%, 20%
3	E	214	76%, 21%

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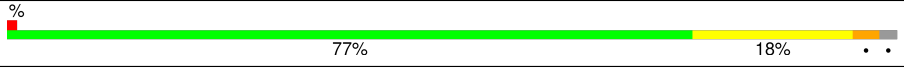
Mol	Chain	Length	Quality of chain
3	G	214	
4	F	226	
4	H	226	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31008 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 Complement C3 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	0	0
			5007	3187	848	957	15			
1	C	642	Total	C	N	O	S	0	0	0
			5007	3187	848	957	15			

- Molecule 2 is a protein called Complement C3 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	903	Total	C	N	O	S	0	0	0
			7213	4572	1213	1390	38			
2	D	903	Total	C	N	O	S	0	0	0
			7213	4572	1213	1390	38			

- Molecule 3 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	214	Total	C	N	O	S	0	0	0
			1640	1027	271	336	6			
3	G	214	Total	C	N	O	S	0	0	0
			1640	1027	271	336	6			

- Molecule 4 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	221	Total	C	N	O	S	0	0	0
			1643	1041	271	324	7			
4	H	221	Total	C	N	O	S	0	0	0
			1643	1041	271	324	7			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

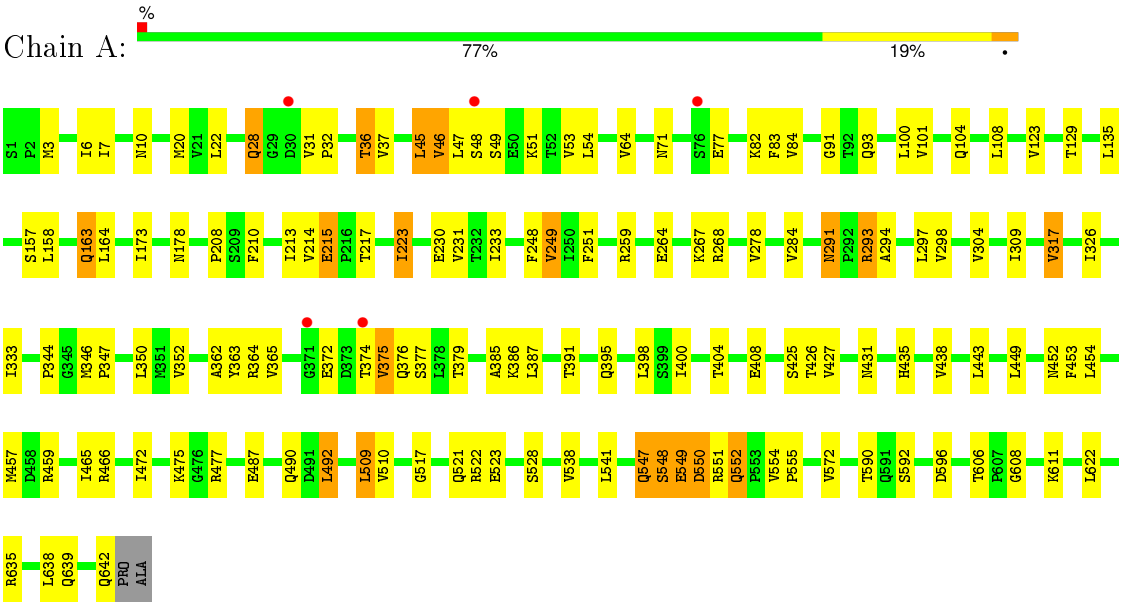
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	C	1	Total Ca 1 1	0	0

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 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.

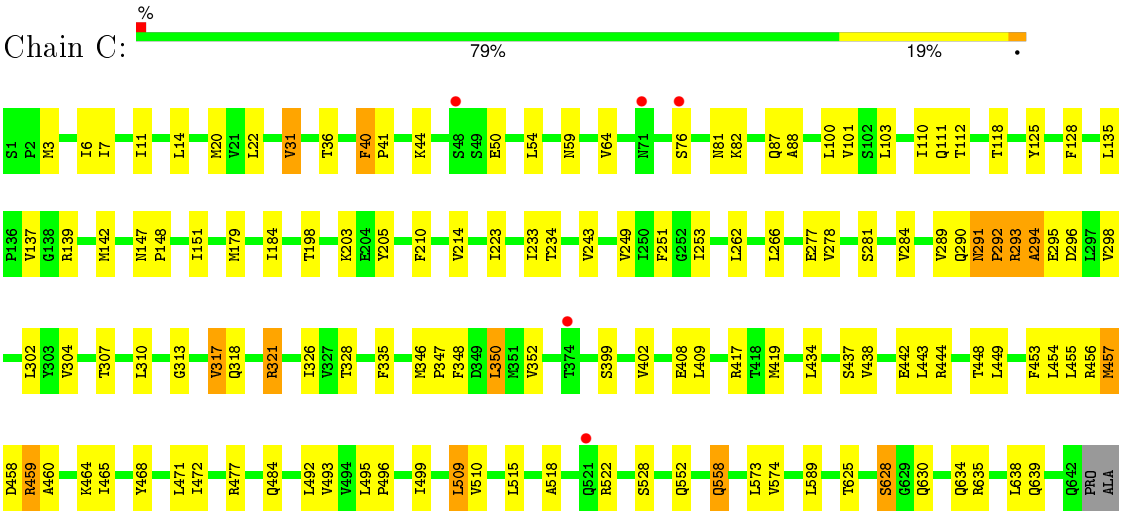
- Molecule 1: Complement C3 beta chain

Chain A:



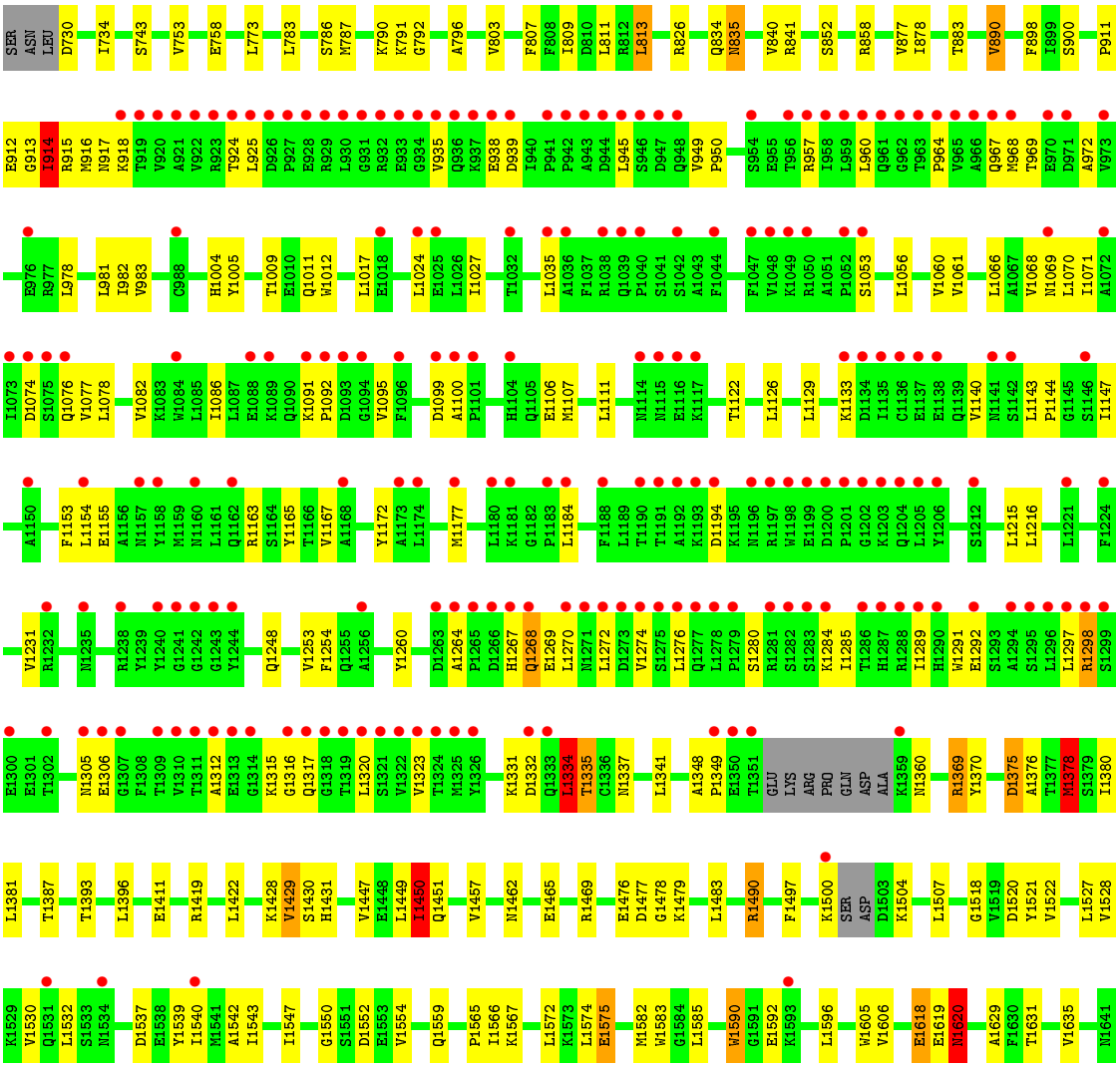
- Molecule 1: Complement C3 beta chain

Chain C:



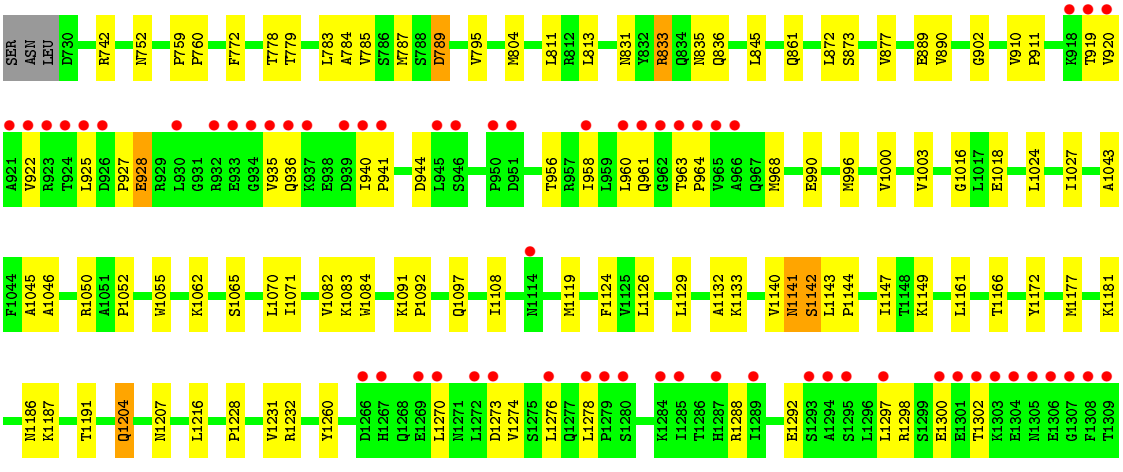
- Molecule 2: Complement C3 alpha chain

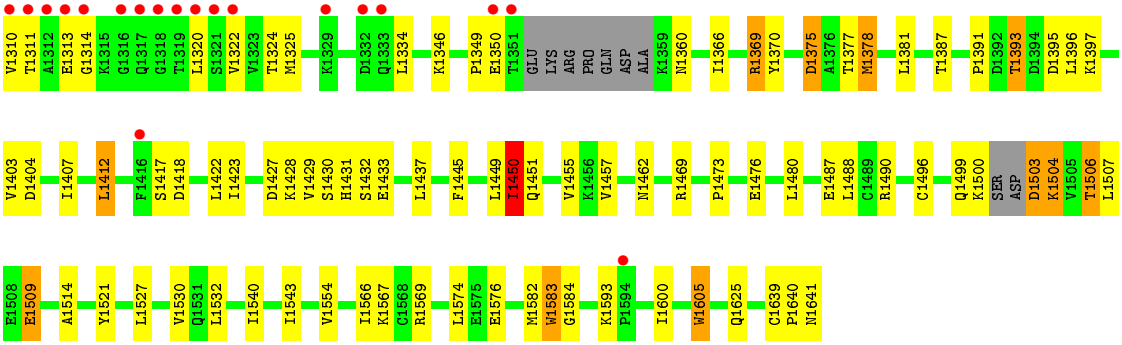
Chain B:



• Molecule 2: Complement C3 alpha chain

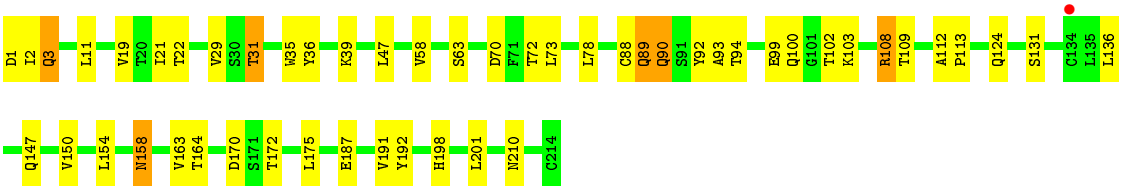
Chain D:





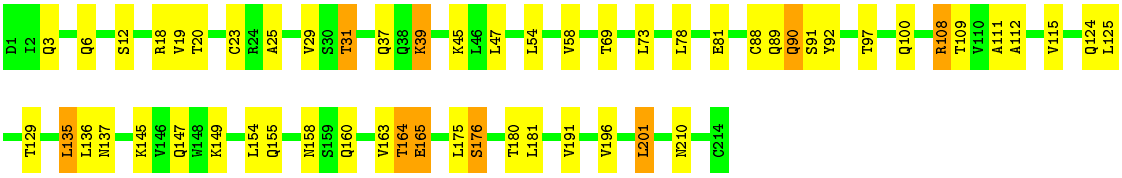
- Molecule 3: Fab light chain

Chain E:



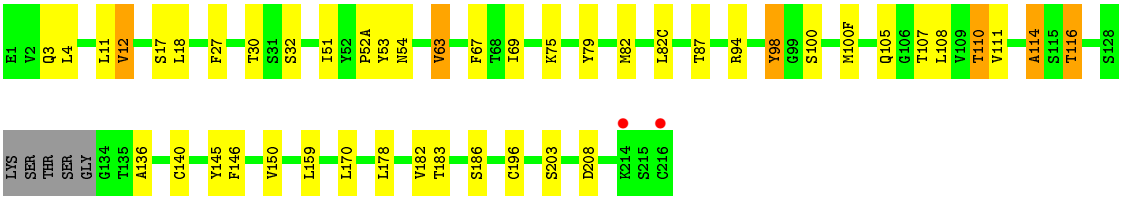
- Molecule 3: Fab light chain

Chain G:



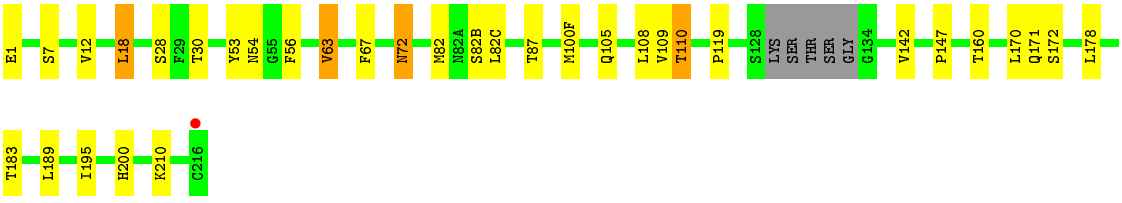
- Molecule 4: Fab heavy chain

Chain F:



- Molecule 4: Fab heavy chain

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	216.44Å 180.42Å 154.58Å 90.00° 115.73° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 49.09 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.10) 100.0 (49.09-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.01	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.214 , 0.282 0.225 , 0.288	Depositor DCC
R_{free} test set	4825 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	48.4	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 31.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 96780 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	31008	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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: CA

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	0.36	0/5108	0.54	0/6940
1	C	0.36	0/5108	0.54	0/6940
2	B	0.37	0/7356	0.51	1/9958 (0.0%)
2	D	0.37	0/7356	0.54	0/9958
3	E	0.37	0/1675	0.53	0/2276
3	G	0.41	0/1675	0.57	0/2276
4	F	0.38	0/1684	0.58	0/2294
4	H	0.40	0/1684	0.60	0/2294
All	All	0.37	0/31646	0.54	1/42936 (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	C	0	1
2	B	0	3
2	D	0	1
4	H	0	1
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1268	GLN	N-CA-C	6.30	128.01	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1267	HIS	Peptide
2	B	1268	GLN	Peptide
2	B	964	PRO	Peptide
1	C	40	PHE	Peptide
2	D	1639	CYS	Peptide
4	H	53	TYR	Peptide

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	5007	0	5068	94	0
1	C	5007	0	5068	104	0
2	B	7213	0	7142	117	0
2	D	7213	0	7140	117	0
3	E	1640	0	1591	30	0
3	G	1640	0	1591	35	0
4	F	1643	0	1593	29	0
4	H	1643	0	1593	28	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
All	All	31008	0	30786	515	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 8.

All (515) 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)
4:F:82:MET:HE2	4:F:82(C):LEU:HD21	1.31	1.07
2:B:1381:LEU:CD2	2:B:1457:VAL:HG12	1.90	1.01
3:E:90:GLN:NE2	3:E:92:TYR:O	1.92	1.00
2:B:1543:ILE:HD12	2:B:1554:VAL:HG21	1.52	0.91
4:H:82:MET:HE2	4:H:82(C):LEU:HD21	1.52	0.91
1:A:249:VAL:HG21	1:A:278:VAL:HG11	1.55	0.88
1:C:151:ILE:HG21	2:D:1297:LEU:HD13	1.55	0.88
4:H:82:MET:CE	4:H:82(C):LEU:HD21	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLN:HE21	1:A:28:GLN:HA	1.43	0.84
4:F:82:MET:CE	4:F:82(C):LEU:HD21	2.07	0.84
2:D:1381:LEU:HD23	2:D:1457:VAL:HG12	1.60	0.84
1:C:443:LEU:HD21	1:C:499:ILE:HG13	1.62	0.80
1:C:20:MET:HE1	1:C:88:ALA:HB2	1.63	0.80
2:B:1572:LEU:HD22	2:B:1574:LEU:HD21	1.65	0.79
3:G:112:ALA:HB1	3:G:201:LEU:HD13	1.64	0.79
4:F:63:VAL:HG13	4:F:67:PHE:HB2	1.66	0.77
1:C:438:VAL:HG13	1:C:449:LEU:HD11	1.65	0.77
2:B:1381:LEU:HD23	2:B:1457:VAL:HG12	1.68	0.76
1:C:290:GLN:C	1:C:292:PRO:CD	2.53	0.76
1:C:293:ARG:CG	1:C:293:ARG:HH11	1.99	0.75
2:B:1543:ILE:CD1	2:B:1554:VAL:HG21	2.15	0.75
1:C:293:ARG:HG2	1:C:293:ARG:HH11	1.51	0.75
1:A:438:VAL:HG11	1:A:449:LEU:HD21	1.67	0.75
3:G:147:GLN:CD	3:G:154:LEU:HD11	2.07	0.74
4:F:82:MET:HE2	4:F:82(C):LEU:CD2	2.16	0.72
1:C:291:ASN:N	1:C:292:PRO:CD	2.53	0.72
1:C:290:GLN:O	1:C:292:PRO:HD2	1.89	0.72
2:D:785:VAL:HG22	2:D:795:VAL:HG22	1.72	0.71
3:G:29:VAL:HG13	3:G:92:TYR:HB2	1.71	0.71
3:G:180:THR:O	3:G:181:LEU:HD13	1.91	0.71
2:B:1543:ILE:HD12	2:B:1554:VAL:CG2	2.20	0.71
1:C:290:GLN:C	1:C:292:PRO:HD2	2.12	0.70
1:C:293:ARG:HG2	1:C:293:ARG:NH1	2.04	0.70
2:D:1527:LEU:HD21	2:D:1530:VAL:HG22	1.74	0.69
1:A:108:LEU:CD2	1:A:129:THR:HG22	2.22	0.69
2:D:811:LEU:HG	2:D:813:LEU:HD13	1.77	0.67
1:C:290:GLN:C	1:C:292:PRO:HD3	2.15	0.67
2:B:925:LEU:HD22	2:B:1312:ALA:HB2	1.77	0.67
2:D:1504:LYS:HG2	2:D:1504:LYS:O	1.93	0.67
1:A:6:ILE:O	1:A:6:ILE:HD12	1.94	0.66
2:B:1369:ARG:HA	2:B:1429:VAL:CG2	2.26	0.66
1:A:347:PRO:HG2	1:C:492:LEU:HD22	1.78	0.66
3:G:137:ASN:HD21	4:H:183:THR:HG21	1.61	0.66
2:B:1068:VAL:HG23	2:B:1069:ASN:HD22	1.60	0.65
1:C:249:VAL:CG2	1:C:278:VAL:HG21	2.26	0.65
3:E:2:ILE:HD12	3:E:93:ALA:HB2	1.78	0.65
1:C:465:ILE:HD11	1:C:515:LEU:HD13	1.77	0.65
1:A:231:VAL:HG21	1:A:304:VAL:HG21	1.79	0.65
2:B:1411:GLU:HG2	2:B:1422:LEU:HD12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1543:ILE:HD12	2:D:1554:VAL:HG21	1.79	0.64
2:D:1521:TYR:CZ	2:D:1584:GLY:HA3	2.32	0.64
2:D:1422:LEU:HD12	2:D:1423:ILE:N	2.13	0.64
1:C:40:PHE:CD2	1:C:40:PHE:O	2.51	0.64
3:E:92:TYR:O	3:E:93:ALA:HB3	1.97	0.63
2:B:914:ILE:HD13	2:B:915:ARG:H	1.64	0.63
2:B:1528:VAL:HG21	2:B:1559:GLN:HE21	1.64	0.63
1:C:348:PHE:CE2	1:C:350:LEU:HD12	2.34	0.63
1:C:291:ASN:O	1:C:293:ARG:N	2.32	0.63
2:B:1284:LYS:O	2:B:1285:ILE:HD13	1.98	0.63
3:E:29:VAL:O	3:E:29:VAL:CG1	2.47	0.62
2:D:1404:ASP:HA	2:D:1427:ASP:CG	2.20	0.62
3:E:124:GLN:HE22	3:E:131:SER:CB	2.12	0.62
1:C:291:ASN:N	1:C:292:PRO:HD3	2.14	0.62
1:A:249:VAL:CG2	1:A:278:VAL:HG21	2.30	0.62
1:C:253:ILE:HD11	1:C:262:LEU:HD11	1.80	0.62
3:G:160:GLN:HE22	4:H:171:GLN:HA	1.64	0.62
4:H:63:VAL:HG21	4:H:67:PHE:CD2	2.35	0.62
1:A:268:ARG:HB2	2:B:1378:MET:HE3	1.81	0.62
2:B:1381:LEU:HD21	2:B:1457:VAL:HG12	1.79	0.61
2:D:910:VAL:HG13	2:D:911:PRO:HD2	1.81	0.61
1:C:249:VAL:HG21	1:C:278:VAL:HG21	1.81	0.61
1:A:248:PHE:HE2	1:A:309:ILE:HD12	1.64	0.61
1:A:346:MET:CE	1:A:454:LEU:HD23	2.30	0.61
1:C:100:LEU:HD21	1:C:638:LEU:HD23	1.82	0.61
1:C:573:LEU:HD23	2:D:784:ALA:HB2	1.83	0.61
2:B:835:ASN:HB3	4:F:54:ASN:HD21	1.66	0.60
1:A:346:MET:HE1	1:A:454:LEU:HD23	1.84	0.60
2:B:967:GLN:O	2:B:969:THR:N	2.35	0.60
3:E:29:VAL:HG12	3:E:29:VAL:O	2.01	0.60
2:D:1387:THR:HG23	2:D:1451:GLN:H	1.65	0.60
1:A:223:ILE:HG23	1:A:326:ILE:CG2	2.32	0.60
2:B:1507:LEU:HD11	2:B:1629:ALA:HB1	1.84	0.59
2:B:1447:VAL:HG13	2:B:1450:ILE:HG22	1.84	0.59
3:E:36:TYR:OH	3:E:89:GLN:NE2	2.35	0.59
1:A:251:PHE:CE1	1:A:304:VAL:HG22	2.38	0.59
2:B:1056:LEU:O	2:B:1060:VAL:HG23	2.03	0.59
1:C:214:VAL:HG12	1:C:233:ILE:HD12	1.84	0.59
4:F:145:TYR:CE2	4:F:150:VAL:HG23	2.37	0.59
1:A:572:VAL:HG12	2:B:753:VAL:HG22	1.83	0.59
4:F:12:VAL:HG23	4:F:111:VAL:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:ARG:O	1:C:295:GLU:N	2.36	0.59
3:G:164:THR:HG23	3:G:165:GLU:O	2.02	0.59
2:B:1370:TYR:N	2:B:1430:SER:O	2.35	0.59
1:A:365:VAL:H	1:A:379:THR:HG22	1.67	0.59
1:A:391:THR:HG22	1:A:398:LEU:HD11	1.83	0.59
2:D:1521:TYR:CE2	2:D:1584:GLY:HA3	2.38	0.58
1:C:210:PHE:CE1	1:C:317:VAL:CG1	2.87	0.58
3:G:54:LEU:HD11	3:G:58:VAL:CG1	2.33	0.58
1:A:293:ARG:O	1:A:294:ALA:C	2.41	0.58
2:D:1274:VAL:HG13	2:D:1311:THR:O	2.03	0.58
2:D:919:THR:HG21	2:D:922:VAL:HG13	1.85	0.58
3:E:112:ALA:HB1	3:E:201:LEU:CD1	2.34	0.58
1:C:223:ILE:HD11	1:C:328:THR:HG22	1.85	0.58
3:G:29:VAL:HG12	3:G:29:VAL:O	2.03	0.58
2:D:1065:SER:OG	2:D:1132:ALA:HB2	2.03	0.57
2:B:1518:GLY:HA3	2:B:1585:LEU:HD22	1.86	0.57
3:G:31:THR:CG2	3:G:31:THR:O	2.52	0.57
1:C:36:THR:HG23	1:C:87:GLN:HB3	1.87	0.57
3:E:163:VAL:HG22	3:E:175:LEU:HD12	1.86	0.57
4:F:63:VAL:HG22	4:F:67:PHE:CG	2.40	0.57
2:B:1155:GLU:O	2:B:1184:LEU:HD21	2.05	0.57
2:D:1082:VAL:HG13	2:D:1129:LEU:CD2	2.34	0.57
1:A:350:LEU:HD12	1:A:400:ILE:HD13	1.86	0.57
2:B:1334:LEU:HG	2:B:1335:THR:HG23	1.86	0.57
2:D:1381:LEU:CD2	2:D:1457:VAL:HG12	2.33	0.56
2:D:1055:TRP:CE2	2:D:1108:ILE:HG22	2.40	0.56
1:C:3:MET:HE3	1:C:522:ARG:HG2	1.87	0.56
1:C:249:VAL:HG21	1:C:278:VAL:HG11	1.85	0.56
2:D:1393:THR:HG22	2:D:1397:LYS:HD2	1.87	0.56
2:B:1215:LEU:HD21	2:B:1231:VAL:HG22	1.87	0.56
2:D:1543:ILE:CD1	2:D:1554:VAL:HG21	2.35	0.56
1:C:214:VAL:HG12	1:C:233:ILE:CD1	2.36	0.56
1:A:554:VAL:HG13	1:A:555:PRO:HD2	1.88	0.56
2:B:924:THR:HG23	2:B:1317:GLN:HG3	1.88	0.56
1:C:223:ILE:HD13	1:C:298:VAL:CG2	2.35	0.56
2:D:1147:ILE:HG22	2:D:1177:MET:HE2	1.88	0.56
2:D:1147:ILE:CG2	2:D:1177:MET:HE2	2.36	0.55
1:C:484:GLN:OE1	1:C:495:LEU:HD13	2.06	0.55
1:C:573:LEU:CD2	2:D:784:ALA:HB2	2.35	0.55
2:B:1122:THR:HB	2:B:1154:LEU:HD21	1.88	0.55
2:D:1437:LEU:C	2:D:1437:LEU:HD12	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:63:VAL:HG22	4:H:67:PHE:CG	2.41	0.55
1:A:100:LEU:HD21	1:A:638:LEU:HG	1.89	0.55
2:D:877:VAL:HG23	2:D:1480:LEU:HD11	1.89	0.55
1:A:606:THR:HG22	1:A:608:GLY:H	1.72	0.54
3:E:19:VAL:HG21	3:E:78:LEU:HD13	1.89	0.54
1:C:214:VAL:O	1:C:214:VAL:HG23	2.08	0.54
1:A:362:ALA:HB1	1:A:365:VAL:HG21	1.90	0.54
3:E:47:LEU:HA	3:E:58:VAL:HG21	1.88	0.54
1:A:510:VAL:HG22	1:A:528:SER:HB3	1.88	0.54
2:B:1027:ILE:HG22	2:B:1071:ILE:HD13	1.89	0.54
1:A:210:PHE:CZ	1:A:317:VAL:HG13	2.43	0.54
2:D:835:ASN:CB	4:H:54:ASN:ND2	2.71	0.54
1:A:249:VAL:HG21	1:A:278:VAL:HG21	1.89	0.54
2:B:1270:LEU:HD23	2:B:1316:GLY:HA2	1.90	0.54
3:G:6:GLN:O	3:G:100:GLN:NE2	2.41	0.54
3:G:108:ARG:HD3	3:G:109:THR:O	2.08	0.54
1:A:6:ILE:C	1:A:6:ILE:HD12	2.29	0.53
2:B:1375:ASP:CG	2:B:1430:SER:HB2	2.28	0.53
2:D:1082:VAL:HG13	2:D:1129:LEU:HD22	1.90	0.53
1:C:472:ILE:HG12	1:C:509:LEU:HD22	1.89	0.53
1:A:84:VAL:HG13	1:A:101:VAL:HG21	1.89	0.53
1:C:6:ILE:CG2	1:C:20:MET:HE2	2.37	0.53
1:C:293:ARG:O	1:C:294:ALA:C	2.46	0.53
2:D:1126:LEU:HD21	2:D:1177:MET:HE1	1.90	0.53
4:H:54:ASN:HD22	4:H:56:PHE:HB2	1.73	0.53
4:F:87:THR:HG23	4:F:110:THR:HA	1.91	0.53
4:F:17:SER:HB2	4:H:72:ASN:HD21	1.73	0.53
4:H:87:THR:HG23	4:H:110:THR:HA	1.90	0.53
2:D:1370:TYR:O	2:D:1431:HIS:HB2	2.08	0.53
2:D:964:PRO:HB3	2:D:1270:LEU:HD11	1.89	0.53
2:D:1369:ARG:HG2	2:D:1430:SER:O	2.09	0.53
1:A:268:ARG:HB2	2:B:1378:MET:CE	2.39	0.53
2:B:773:LEU:HD13	2:B:803:VAL:HG22	1.91	0.53
1:C:6:ILE:HG21	1:C:20:MET:HE2	1.91	0.53
2:D:845:LEU:HD22	2:D:889:GLU:HG2	1.91	0.53
1:C:307:THR:HG23	1:C:318:GLN:HG2	1.90	0.52
1:C:151:ILE:CG2	2:D:1297:LEU:HD13	2.34	0.52
1:A:7:ILE:CG2	1:A:622:LEU:HD22	2.39	0.52
2:B:898:PHE:HB2	4:F:98:TYR:HA	1.91	0.52
2:D:940:ILE:HG21	2:D:1322:VAL:HG21	1.91	0.52
1:A:108:LEU:HD21	1:A:129:THR:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1514:ALA:HB2	2:D:1583:TRP:CZ2	2.45	0.52
1:A:213:ILE:HG22	1:A:215:GLU:HG3	1.92	0.52
4:F:159:LEU:HD21	4:F:182:VAL:HG21	1.91	0.52
2:B:925:LEU:HD13	2:B:1272:LEU:HD13	1.91	0.52
2:B:978:LEU:HB3	2:B:981:LEU:HD12	1.90	0.52
1:A:547:GLN:O	1:A:549:GLU:N	2.43	0.52
2:B:1272:LEU:HB2	2:B:1289:ILE:HD12	1.91	0.52
2:D:831:ASN:OD1	2:D:833:ARG:HB2	2.10	0.52
4:H:63:VAL:CG2	4:H:67:PHE:CD2	2.93	0.52
4:H:72:ASN:HD22	4:H:72:ASN:C	2.12	0.52
3:G:37:GLN:HB2	3:G:47:LEU:HD11	1.92	0.52
2:B:1126:LEU:HA	2:B:1129:LEU:HD12	1.92	0.52
2:B:1035:LEU:HD21	2:B:1077:VAL:HG11	1.91	0.52
1:C:210:PHE:CE1	1:C:317:VAL:HG13	2.46	0.51
2:B:1053:SER:HA	2:B:1100:ALA:HB3	1.91	0.51
2:B:1483:LEU:HD13	2:B:1565:PRO:HG3	1.92	0.51
2:B:1522:VAL:HG22	2:B:1583:TRP:HB3	1.92	0.51
1:A:472:ILE:HG12	1:A:509:LEU:HD22	1.91	0.51
1:C:40:PHE:CG	1:C:40:PHE:O	2.63	0.51
2:D:958:ILE:HD12	2:D:1300:GLU:HB2	1.91	0.51
1:A:374:THR:HG22	1:C:448:THR:HB	1.93	0.51
2:B:811:LEU:HG	2:B:813:LEU:HD13	1.92	0.51
2:D:956:THR:HA	2:D:1324:THR:HG22	1.92	0.51
2:D:1532:LEU:HD23	2:D:1569:ARG:NH1	2.26	0.51
2:B:1280:SER:HB2	2:B:1306:GLU:HG3	1.93	0.51
2:B:1507:LEU:HD11	2:B:1629:ALA:CB	2.41	0.51
2:B:960:LEU:HD21	2:B:1320:LEU:HD13	1.91	0.51
2:B:1337:ASN:HD21	2:B:1465:GLU:HG2	1.76	0.51
3:E:147:GLN:OE1	3:E:154:LEU:HD11	2.11	0.51
1:C:291:ASN:O	1:C:292:PRO:C	2.49	0.51
1:A:438:VAL:CG1	1:A:449:LEU:HD11	2.41	0.51
1:A:53:VAL:HG23	1:A:53:VAL:O	2.11	0.51
1:C:6:ILE:HG22	1:C:22:LEU:HD23	1.91	0.51
1:A:32:PRO:HA	1:A:53:VAL:HG12	1.92	0.51
1:A:350:LEU:HD13	1:A:400:ILE:HG21	1.93	0.50
1:C:434:LEU:HD13	1:C:468:TYR:CE1	2.46	0.50
1:C:112:THR:HG22	1:C:125:TYR:HB3	1.92	0.50
3:G:90:GLN:NE2	3:G:97:THR:OG1	2.44	0.50
4:H:108:LEU:HD22	4:H:110:THR:HG22	1.94	0.50
2:B:1522:VAL:HG22	2:B:1583:TRP:CB	2.42	0.50
2:D:1027:ILE:HG22	2:D:1071:ILE:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:LEU:HG	2:D:1378:MET:HE1	1.93	0.50
1:C:135:LEU:HD22	2:D:789:ASP:O	2.12	0.49
1:A:249:VAL:HG21	1:A:278:VAL:CG1	2.36	0.49
2:D:1527:LEU:HD21	2:D:1530:VAL:CG2	2.42	0.49
2:D:783:LEU:HD12	2:D:784:ALA:N	2.27	0.49
1:A:374:THR:O	1:A:376:GLN:N	2.46	0.49
3:G:136:LEU:HD12	3:G:136:LEU:N	2.27	0.49
4:H:82:MET:HE1	4:H:82(C):LEU:HD21	1.91	0.49
2:D:742:ARG:N	2:D:902:GLY:O	2.44	0.49
3:E:92:TYR:O	3:E:93:ALA:CB	2.61	0.49
1:A:443:LEU:HD11	1:A:449:LEU:HD22	1.93	0.49
1:A:264:GLU:HB3	1:A:284:VAL:HG13	1.93	0.49
2:B:1539:TYR:CD1	2:B:1574:LEU:HD12	2.48	0.49
3:G:112:ALA:HB1	3:G:201:LEU:CD1	2.39	0.49
4:H:195:ILE:HG22	4:H:210:LYS:HA	1.93	0.49
4:F:12:VAL:HG21	4:F:82(C):LEU:HD13	1.94	0.49
2:B:1012:TRP:HB3	2:B:1017:LEU:HD12	1.95	0.49
2:D:1119:MET:HG3	2:D:1161:LEU:HD21	1.94	0.49
2:B:1068:VAL:HG23	2:B:1069:ASN:ND2	2.27	0.49
2:B:925:LEU:HD22	2:B:1312:ALA:CB	2.41	0.49
2:B:981:LEU:O	2:B:983:VAL:HG23	2.13	0.48
3:E:22:THR:HG22	3:E:72:THR:HG22	1.95	0.48
2:D:1583:TRP:HB2	2:D:1605:TRP:H	1.78	0.48
1:A:459:ARG:CD	1:C:458:ASP:HB3	2.43	0.48
3:G:154:LEU:HD23	3:G:155:GLN:N	2.29	0.48
2:D:1527:LEU:HD22	2:D:1574:LEU:HB3	1.95	0.48
1:A:452:ASN:HB3	1:A:492:LEU:HD21	1.96	0.48
4:F:116:THR:HG23	4:F:203:SER:HB3	1.95	0.48
2:D:1450:ILE:HD11	2:D:1473:PRO:CD	2.42	0.48
4:H:63:VAL:HG13	4:H:67:PHE:HB2	1.95	0.48
1:C:243:VAL:HG13	1:C:310:LEU:HD22	1.95	0.48
1:C:137:VAL:HG21	1:C:139:ARG:NH1	2.27	0.48
1:C:14:LEU:HD11	1:C:103:LEU:HD12	1.94	0.48
2:D:877:VAL:HG22	2:D:1451:GLN:NE2	2.28	0.48
1:A:164:LEU:O	2:B:787:MET:HG2	2.13	0.48
4:F:69:ILE:HA	4:F:79:TYR:O	2.14	0.48
1:C:179:MET:HG3	1:C:203:LYS:HA	1.96	0.48
2:B:1133:LYS:NZ	2:B:1147:ILE:HD12	2.28	0.48
2:D:1543:ILE:HD13	2:D:1554:VAL:HG11	1.96	0.48
2:D:1375:ASP:CG	2:D:1430:SER:HB2	2.34	0.48
2:B:1143:LEU:HB3	2:B:1144:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:ILE:HB	1:C:198:THR:OG1	2.13	0.48
2:D:1141:ASN:O	2:D:1142:SER:CB	2.62	0.48
3:E:3:GLN:HE21	3:E:3:GLN:CA	2.26	0.48
2:B:877:VAL:HG22	2:B:1451:GLN:CG	2.44	0.48
1:C:7:ILE:N	1:C:7:ILE:HD12	2.29	0.48
1:C:118:THR:HG23	1:C:205:TYR:CE2	2.49	0.48
2:B:807:PHE:CE1	2:B:840:VAL:HG21	2.49	0.48
1:A:45:LEU:C	1:A:45:LEU:HD22	2.35	0.48
2:D:835:ASN:HB2	4:H:54:ASN:ND2	2.28	0.48
2:D:833:ARG:HH11	2:D:836:GLN:NE2	2.12	0.48
4:F:51:ILE:O	4:F:52(A):PRO:HD3	2.13	0.48
2:D:1274:VAL:HG12	2:D:1276:LEU:CD1	2.44	0.47
1:C:6:ILE:HG21	1:C:20:MET:CE	2.44	0.47
4:H:178:LEU:C	4:H:178:LEU:HD12	2.35	0.47
2:D:927:PRO:O	2:D:928:GLU:HB2	2.14	0.47
1:A:157:SER:O	1:A:158:LEU:HD13	2.14	0.47
1:C:459:ARG:HG3	1:C:460:ALA:N	2.29	0.47
1:A:541:LEU:HD22	2:B:786:SER:HB3	1.96	0.47
2:D:1366:ILE:HD13	2:D:1455:VAL:HG11	1.95	0.47
2:B:949:VAL:HG13	2:B:950:PRO:HD2	1.95	0.47
3:G:137:ASN:HD21	4:H:183:THR:CG2	2.26	0.47
3:E:108:ARG:HD3	3:E:109:THR:O	2.14	0.47
2:D:1161:LEU:HD22	2:D:1166:THR:HG21	1.97	0.47
2:B:877:VAL:HG22	2:B:1451:GLN:HG3	1.96	0.47
1:C:281:SER:OG	1:C:284:VAL:HG23	2.15	0.47
3:E:35:TRP:CE3	3:E:73:LEU:HD12	2.49	0.47
3:G:19:VAL:CG2	3:G:78:LEU:HD22	2.45	0.47
2:D:1407:ILE:HG22	2:D:1412:LEU:HD13	1.96	0.47
3:G:137:ASN:ND2	4:H:183:THR:HG21	2.27	0.47
2:B:1107:MET:O	2:B:1248:GLN:HG2	2.14	0.47
2:D:1143:LEU:HB3	2:D:1144:PRO:HD3	1.96	0.47
4:F:12:VAL:HG21	4:F:82(C):LEU:CD1	2.45	0.47
2:D:960:LEU:CD2	2:D:1320:LEU:HD13	2.45	0.47
1:A:251:PHE:CD1	1:A:304:VAL:HG22	2.48	0.47
3:G:135:LEU:HD22	3:G:136:LEU:N	2.29	0.47
3:G:175:LEU:HD23	3:G:176:SER:N	2.30	0.47
1:A:217:THR:HG23	1:A:230:GLU:O	2.15	0.47
2:B:1024:LEU:HD11	2:B:1070:LEU:HB3	1.96	0.47
1:A:214:VAL:HG13	1:A:233:ILE:CD1	2.44	0.47
1:A:541:LEU:HG	2:B:796:ALA:HB2	1.96	0.47
2:B:1163:ARG:O	2:B:1167:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:TYR:CD1	1:A:364:ARG:HG2	2.50	0.47
2:B:1530:VAL:HG12	2:B:1532:LEU:CD1	2.45	0.47
2:B:1631:THR:O	2:B:1635:VAL:HG23	2.14	0.47
1:A:291:ASN:N	1:A:291:ASN:OD1	2.47	0.47
2:D:960:LEU:HD23	2:D:1320:LEU:HD13	1.97	0.46
1:C:455:LEU:HD12	1:C:456:ARG:H	1.80	0.46
2:B:1370:TYR:CG	2:B:1376:ALA:HB2	2.51	0.46
2:B:1095:VAL:HG22	2:B:1153:PHE:CE2	2.50	0.46
2:B:1009:THR:HB	2:B:1011:GLN:HE21	1.79	0.46
3:E:191:VAL:HG22	3:E:210:ASN:OD1	2.15	0.46
2:B:1380:ILE:N	2:B:1380:ILE:HD12	2.31	0.46
2:D:1055:TRP:CD2	2:D:1108:ILE:HG22	2.51	0.46
2:B:1004:HIS:HB2	2:B:1066:LEU:HD21	1.98	0.46
2:B:972:ALA:HB1	2:B:1005:TYR:OH	2.15	0.46
2:B:1297:LEU:HD23	2:B:1298:ARG:N	2.30	0.46
1:A:346:MET:HE1	1:A:435:HIS:HB3	1.98	0.46
1:C:82:LYS:HZ2	1:C:103:LEU:HD11	1.80	0.46
4:F:63:VAL:CG2	4:F:67:PHE:CD2	2.99	0.46
1:C:214:VAL:HG23	1:C:321:ARG:HB2	1.98	0.46
2:B:1082:VAL:HG13	2:B:1129:LEU:HD23	1.98	0.46
2:B:1375:ASP:OD1	2:B:1430:SER:HB2	2.16	0.46
1:A:37:VAL:O	1:A:46:VAL:HG13	2.16	0.46
2:D:1530:VAL:HG23	2:D:1576:GLU:HG2	1.98	0.46
2:D:835:ASN:HB3	4:H:54:ASN:ND2	2.30	0.46
1:A:548:SER:O	1:A:549:GLU:O	2.34	0.46
2:D:1500:LYS:HG2	2:D:1503:ASP:HB2	1.98	0.46
3:G:29:VAL:HG13	3:G:92:TYR:CB	2.42	0.45
1:A:223:ILE:HD13	1:A:298:VAL:CG2	2.46	0.45
1:A:3:MET:HE3	1:A:522:ARG:CG	2.47	0.45
2:D:778:THR:OG1	2:D:779:THR:N	2.49	0.45
2:D:872:LEU:HD23	2:D:873:SER:N	2.31	0.45
1:C:495:LEU:HD12	1:C:496:PRO:HD2	1.97	0.45
2:D:1204:GLN:HA	2:D:1207:ASN:ND2	2.31	0.45
1:C:471:LEU:HD12	1:C:471:LEU:N	2.32	0.45
3:G:163:VAL:HG12	3:G:164:THR:O	2.16	0.45
2:D:1045:ALA:HB2	2:D:1052:PRO:HA	1.97	0.45
2:D:1540:ILE:HD12	2:D:1540:ILE:N	2.31	0.45
1:A:47:LEU:O	1:A:47:LEU:HD23	2.17	0.45
1:C:210:PHE:CZ	1:C:317:VAL:HG12	2.51	0.45
2:D:1126:LEU:HD11	2:D:1177:MET:CE	2.46	0.45
2:D:1133:LYS:HA	2:D:1143:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:119:PRO:HB2	4:H:142:VAL:HG13	1.97	0.45
1:A:457:MET:HE1	1:A:465:ILE:CG1	2.47	0.45
1:C:335:PHE:CD2	1:C:419:MET:HB3	2.50	0.45
4:H:147:PRO:O	4:H:200:HIS:HE1	2.00	0.45
2:B:1086:ILE:HD12	2:B:1140:VAL:HG11	1.99	0.45
1:C:628:SER:HB2	1:C:630:GLN:OE1	2.17	0.45
4:H:30:THR:HG22	4:H:30:THR:O	2.17	0.45
1:C:6:ILE:HB	1:C:20:MET:HE2	1.99	0.45
2:D:872:LEU:HD11	2:D:1418:ASP:CG	2.37	0.45
1:A:590:THR:HG22	1:A:592:SER:H	1.80	0.45
2:D:1582:MET:HA	2:D:1605:TRP:O	2.16	0.45
2:B:1521:TYR:O	2:B:1583:TRP:HB2	2.16	0.45
1:A:459:ARG:CZ	1:C:458:ASP:HB2	2.47	0.45
2:B:852:SER:HB3	2:B:878:ILE:HG22	1.98	0.45
1:A:267:LYS:HG3	1:A:278:VAL:HG23	1.99	0.45
1:A:350:LEU:CD2	1:A:352:VAL:HG22	2.46	0.45
2:D:920:VAL:HG11	2:D:941:PRO:O	2.16	0.45
4:F:30:THR:HG23	4:F:53:TYR:HA	1.98	0.45
2:B:809:ILE:HD13	2:B:890:VAL:HG23	1.99	0.45
1:A:426:THR:HG21	1:A:431:ASN:HA	1.99	0.45
1:C:348:PHE:HE2	1:C:350:LEU:HD12	1.79	0.45
1:A:487:GLU:H	1:A:490:GLN:HE21	1.65	0.44
2:D:759:PRO:HA	2:D:760:PRO:HD3	1.85	0.44
2:B:1348:ALA:HB1	2:B:1349:PRO:CD	2.47	0.44
4:F:114:ALA:HB3	4:F:146:PHE:CE1	2.52	0.44
2:D:1496:CYS:O	2:D:1600:ILE:HG22	2.17	0.44
2:B:1582:MET:HA	2:B:1605:TRP:O	2.17	0.44
2:B:734:ILE:HD12	2:B:900:SER:HB3	1.98	0.44
1:C:31:VAL:HG13	1:C:54:LEU:HB2	2.00	0.44
2:B:925:LEU:CD1	2:B:1272:LEU:HD13	2.48	0.44
1:A:350:LEU:HD12	1:A:400:ILE:CD1	2.47	0.44
1:C:455:LEU:HD11	1:C:457:MET:HG2	1.99	0.44
2:D:1369:ARG:HD3	2:D:1433:GLU:O	2.17	0.44
2:B:945:LEU:HD12	2:B:1305:ASN:CG	2.38	0.44
2:B:1260:TYR:O	2:B:1264:ALA:HB2	2.18	0.44
2:D:1083:LYS:HG3	2:D:1140:VAL:HG13	1.99	0.44
1:A:77:GLU:OE1	1:A:82:LYS:NZ	2.49	0.44
1:C:253:ILE:N	1:C:253:ILE:HD12	2.33	0.44
1:C:352:VAL:HG21	1:C:402:VAL:HG11	2.00	0.44
1:A:375:VAL:HG12	1:A:375:VAL:O	2.18	0.44
1:C:453:PHE:HB2	1:C:493:VAL:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:VAL:HG22	1:A:528:SER:CB	2.47	0.43
2:B:1061:VAL:HG13	2:B:1078:LEU:HD11	2.00	0.43
4:F:178:LEU:HD12	4:F:178:LEU:C	2.37	0.43
3:G:108:ARG:NH1	3:G:111:ALA:HB2	2.33	0.43
2:B:1253:VAL:HG13	2:B:1254:PHE:CD2	2.53	0.43
1:A:386:LYS:O	1:A:387:LEU:HD23	2.18	0.43
3:E:170:ASP:O	3:E:172:THR:HG23	2.18	0.43
1:C:111:GLN:NE2	1:C:574:VAL:HG11	2.33	0.43
2:B:1527:LEU:HD12	2:B:1540:ILE:O	2.18	0.43
2:D:1043:ALA:HB2	2:D:1084:TRP:CD2	2.54	0.43
2:D:1091:LYS:HE3	2:D:1097:GLN:OE1	2.19	0.43
3:G:147:GLN:HG2	3:G:154:LEU:HD21	2.00	0.43
2:B:1527:LEU:HD23	2:B:1575:GLU:O	2.19	0.43
1:C:313:GLY:HA2	2:D:1423:ILE:HD11	2.00	0.43
3:E:21:ILE:HG12	3:E:102:THR:HG21	2.00	0.43
2:D:1369:ARG:NH2	2:D:1430:SER:HB3	2.34	0.43
2:B:1091:LYS:HB3	2:B:1092:PRO:HD2	2.01	0.43
3:G:29:VAL:CG1	3:G:29:VAL:O	2.66	0.43
2:D:925:LEU:HD23	2:D:936:GLN:NE2	2.33	0.43
3:E:147:GLN:CD	3:E:154:LEU:HD11	2.39	0.43
1:C:302:LEU:HD21	1:C:326:ILE:HD11	2.01	0.43
1:C:147:ASN:HB2	1:C:148:PRO:CD	2.48	0.43
2:B:1520:ASP:O	2:B:1550:GLY:HA3	2.19	0.43
4:F:27:PHE:CE2	4:F:94:ARG:HD2	2.53	0.43
3:G:136:LEU:CD1	3:G:136:LEU:N	2.82	0.43
2:B:916:MET:HE2	2:B:916:MET:HA	2.00	0.43
1:C:291:ASN:ND2	1:C:296:ASP:OD2	2.51	0.43
1:A:347:PRO:HD3	1:C:492:LEU:HB3	2.00	0.43
1:A:549:GLU:O	1:A:550:ASP:C	2.58	0.43
4:F:94:ARG:O	4:F:100(F):MET:HA	2.19	0.43
2:D:1187:LYS:O	2:D:1191:THR:OG1	2.34	0.43
2:B:1111:LEU:HD12	2:B:1165:TYR:HE2	1.84	0.43
2:B:1490:ARG:HG2	2:B:1590:TRP:CZ2	2.54	0.43
1:C:573:LEU:HD23	2:D:784:ALA:CB	2.49	0.42
1:A:453:PHE:O	1:A:492:LEU:HD23	2.19	0.42
1:A:3:MET:HE3	1:A:522:ARG:HG2	2.01	0.42
4:H:18:LEU:HD12	4:H:109:VAL:HG13	2.01	0.42
4:F:63:VAL:CG1	4:F:67:PHE:HB2	2.45	0.42
2:D:919:THR:CG2	2:D:922:VAL:HG13	2.49	0.42
1:C:137:VAL:HG21	1:C:139:ARG:CZ	2.49	0.42
1:A:538:VAL:HG12	2:B:791:LYS:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:113:PRO:HD3	3:E:198:HIS:CD2	2.53	0.42
4:F:3:GLN:C	4:F:4:LEU:HD12	2.39	0.42
3:G:25:ALA:HB3	3:G:69:THR:HA	1.99	0.42
3:E:136:LEU:HD12	3:E:136:LEU:N	2.35	0.42
2:B:914:ILE:HG23	2:B:915:ARG:N	2.34	0.42
3:E:11:LEU:C	3:E:11:LEU:HD12	2.40	0.42
2:D:960:LEU:O	2:D:1297:LEU:HA	2.19	0.42
1:C:36:THR:HG22	1:C:87:GLN:O	2.20	0.42
1:C:110:ILE:HD13	1:C:184:ILE:O	2.20	0.42
1:A:20:MET:CE	1:A:22:LEU:HD21	2.49	0.42
2:D:936:GLN:O	2:D:1311:THR:HG23	2.19	0.42
4:F:63:VAL:HG21	4:F:67:PHE:CD2	2.54	0.42
2:B:1552:ASP:OD1	2:B:1596:LEU:HD13	2.19	0.42
3:G:115:VAL:HG22	3:G:196:VAL:HG21	2.01	0.42
1:A:492:LEU:HB3	1:C:347:PRO:HD3	2.02	0.42
2:B:1547:ILE:HG12	2:B:1631:THR:HG23	2.00	0.42
1:A:377:SER:O	1:A:385:ALA:HB1	2.20	0.42
2:D:1228:PRO:O	2:D:1232:ARG:HB2	2.19	0.42
3:E:150:VAL:HG22	3:E:192:TYR:CD2	2.55	0.42
3:E:31:THR:O	3:E:31:THR:HG23	2.18	0.42
1:C:50:GLU:HB3	1:C:64:VAL:HG13	2.02	0.42
1:C:251:PHE:CD1	1:C:304:VAL:HG22	2.55	0.42
2:D:1119:MET:HE2	2:D:1161:LEU:HD11	2.00	0.42
2:B:918:LYS:H	2:B:1323:VAL:HG13	1.85	0.42
2:B:1447:VAL:CG1	2:B:1450:ILE:HG22	2.48	0.41
2:B:1074:ASP:HB3	2:B:1077:VAL:HG23	2.01	0.41
1:C:346:MET:HE1	1:C:454:LEU:HD23	2.01	0.41
1:C:589:LEU:HG	2:D:795:VAL:HG21	2.01	0.41
2:D:1543:ILE:HD12	2:D:1554:VAL:CG2	2.49	0.41
1:A:459:ARG:NE	1:C:458:ASP:HB3	2.35	0.41
1:A:123:VAL:CG2	1:A:173:ILE:HD11	2.50	0.41
1:A:135:LEU:HD23	2:B:792:GLY:CA	2.49	0.41
1:C:455:LEU:HB2	1:C:468:TYR:OH	2.21	0.41
2:B:1532:LEU:N	2:B:1532:LEU:HD12	2.36	0.41
1:A:333:ILE:HD11	1:A:404:THR:HG23	2.03	0.41
2:D:1504:LYS:CG	2:D:1504:LYS:O	2.64	0.41
1:A:438:VAL:CG1	1:A:449:LEU:HD21	2.44	0.41
1:C:14:LEU:HD11	1:C:103:LEU:CD1	2.50	0.41
2:D:1003:VAL:CG1	2:D:1070:LEU:HD13	2.50	0.41
2:B:1341:LEU:HD13	2:B:1457:VAL:HG11	2.03	0.41
1:C:6:ILE:CB	1:C:20:MET:HE2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:783:LEU:HD12	2:D:784:ALA:H	1.85	0.41
3:G:54:LEU:HD11	3:G:58:VAL:HG11	2.02	0.41
3:E:112:ALA:HB1	3:E:201:LEU:HD13	2.01	0.41
4:H:30:THR:O	4:H:30:THR:CG2	2.68	0.41
2:D:1391:PRO:HB2	2:D:1396:LEU:HD11	2.02	0.41
1:A:427:VAL:HB	1:A:523:GLU:HG3	2.02	0.41
1:C:408:GLU:C	1:C:409:LEU:HD12	2.41	0.41
3:G:191:VAL:HG22	3:G:210:ASN:OD1	2.20	0.41
2:D:1506:THR:N	2:D:1509:GLU:HG3	2.36	0.41
4:H:63:VAL:HG22	4:H:67:PHE:CD1	2.56	0.41
2:B:1396:LEU:HD12	2:B:1419:ARG:NH1	2.35	0.41
2:D:990:GLU:OE2	2:D:1046:ALA:HB2	2.20	0.41
2:D:1231:VAL:HG21	2:D:1260:TYR:CE1	2.56	0.41
2:B:1274:VAL:HG12	2:B:1276:LEU:CD1	2.51	0.41
3:E:158:ASN:H	3:E:158:ASN:HD22	1.67	0.41
3:G:147:GLN:CG	3:G:154:LEU:HD11	2.50	0.41
2:B:1528:VAL:CG2	2:B:1542:ALA:HB2	2.51	0.41
2:D:1403:VAL:O	2:D:1404:ASP:HB2	2.21	0.41
3:E:124:GLN:HE22	3:E:131:SER:HB2	1.86	0.41
1:A:344:PRO:HG2	1:A:395:GLN:HE22	1.86	0.41
2:D:996:MET:O	2:D:1000:VAL:HG23	2.20	0.41
2:B:1341:LEU:HD22	2:B:1457:VAL:HG13	2.03	0.41
1:A:83:PHE:CE1	2:B:1017:LEU:HD22	2.56	0.41
2:D:1119:MET:CE	2:D:1161:LEU:HD11	2.51	0.41
1:C:11:ILE:HD11	1:C:635:ARG:CZ	2.50	0.41
3:G:39:LYS:NZ	3:G:81:GLU:O	2.48	0.41
1:C:128:PHE:HB3	2:D:787:MET:HE1	2.01	0.41
1:C:558:GLN:HG3	2:D:772:PHE:CE1	2.56	0.41
2:D:961:GLN:NE2	2:D:963:THR:HG23	2.35	0.41
1:A:347:PRO:CG	1:C:492:LEU:HD22	2.46	0.41
2:B:1147:ILE:HG23	2:B:1177:MET:CE	2.51	0.41
2:B:858:ARG:CZ	2:B:1449:LEU:HD12	2.51	0.41
4:F:12:VAL:CG2	4:F:111:VAL:HG22	2.49	0.40
2:B:1369:ARG:HE	2:B:1430:SER:HB3	1.86	0.40
1:A:297:LEU:HB3	1:A:326:ILE:HD13	2.03	0.40
2:B:1270:LEU:HD12	2:B:1291:TRP:HB2	2.03	0.40
2:B:1530:VAL:HG12	2:B:1532:LEU:HD12	2.03	0.40
1:A:10:ASN:HB3	1:A:635:ARG:HD3	2.02	0.40
4:F:136:ALA:HB2	4:F:186:SER:HB3	2.04	0.40
1:A:36:THR:HG23	1:A:48:SER:CB	2.52	0.40
1:C:289:VAL:HG12	1:C:291:ASN:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:150:VAL:HG13	3:E:192:TYR:CE2	2.56	0.40
1:C:100:LEU:HD12	1:C:101:VAL:H	1.86	0.40
4:F:17:SER:HB2	4:H:72:ASN:ND2	2.35	0.40
2:D:1091:LYS:HB3	2:D:1092:PRO:HD2	2.03	0.40
2:D:1278:LEU:HD22	2:D:1302:THR:HG21	2.03	0.40
2:D:935:VAL:HG11	2:D:1313:GLU:HG3	2.02	0.40
2:D:1310:VAL:HG11	2:D:1320:LEU:CD2	2.51	0.40
2:B:1619:GLU:O	2:B:1620:ASN:CB	2.69	0.40
2:B:1172:TYR:CE1	2:B:1216:LEU:HB3	2.56	0.40
1:C:510:VAL:HG22	1:C:528:SER:HB3	2.04	0.40
1:A:163:GLN:HE21	1:A:163:GLN:HB2	1.68	0.40
2:D:1172:TYR:CE1	2:D:1216:LEU:HB3	2.57	0.40
2:D:1274:VAL:HG12	2:D:1276:LEU:HD11	2.03	0.40
2:D:1062:LYS:HE3	2:D:1124:PHE:CE1	2.57	0.40
3:G:124:GLN:HE21	3:G:129:THR:HG22	1.87	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	640/644 (99%)	595 (93%)	37 (6%)	8 (1%)	15 50
1	C	640/644 (99%)	581 (91%)	48 (8%)	11 (2%)	11 43
2	B	897/915 (98%)	798 (89%)	79 (9%)	20 (2%)	8 36
2	D	897/915 (98%)	809 (90%)	70 (8%)	18 (2%)	9 38
3	E	212/214 (99%)	204 (96%)	8 (4%)	0	100 100
3	G	212/214 (99%)	200 (94%)	12 (6%)	0	100 100
4	F	217/226 (96%)	203 (94%)	12 (6%)	2 (1%)	21 61
4	H	217/226 (96%)	211 (97%)	6 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3932/3998 (98%)	3601 (92%)	272 (7%)	59 (2%)	13 46

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	548	SER
1	A	549	GLU
2	B	913	GLY
2	B	935	VAL
2	B	968	MET
2	B	1497	PHE
1	C	41	PRO
1	C	59	ASN
1	C	292	PRO
1	C	442	GLU
1	C	459	ARG
2	D	1334	LEU
2	D	1360	ASN
2	D	1417	SER
2	D	1476	GLU
2	D	1640	PRO
4	F	98	TYR
1	A	375	VAL
2	B	914	ILE
2	B	1292	GLU
2	B	1429	VAL
2	B	1450	ILE
2	B	1476	GLU
2	B	1478	GLY
2	B	1620	ASN
2	D	928	GLU
2	D	1142	SER
2	D	1292	GLU
2	D	1350	GLU
2	D	1429	VAL
2	D	1432	SER
2	D	1450	ILE
1	A	550	ASP
2	B	911	PRO
2	B	1334	LEU
2	B	1378	MET
2	B	1592	GLU

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Mol	Chain	Res	Type
2	B	1618	GLU
1	C	294	ALA
1	C	518	ALA
2	D	1377	THR
1	A	49	SER
1	A	552	GLN
2	B	1335	THR
1	C	76	SER
1	C	552	GLN
2	D	944	ASP
2	D	1449	LEU
4	F	114	ALA
2	B	1315	LYS
1	C	81	ASN
1	A	91	GLY
2	B	1331	LYS
1	C	291	ASN
2	D	1349	PRO
1	A	517	GLY
2	D	1016	GLY
2	D	1314	GLY
2	B	982	ILE

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	566/567 (100%)	529 (94%)	37 (6%)	21 57
1	C	566/567 (100%)	544 (96%)	22 (4%)	39 75
2	B	799/810 (99%)	749 (94%)	50 (6%)	22 58
2	D	799/810 (99%)	752 (94%)	47 (6%)	24 60
3	E	188/188 (100%)	171 (91%)	17 (9%)	12 41
3	G	188/188 (100%)	165 (88%)	23 (12%)	6 24
4	F	181/185 (98%)	164 (91%)	17 (9%)	11 39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	H	181/185 (98%)	166 (92%)	15 (8%)	14 46
All	All	3468/3500 (99%)	3240 (93%)	228 (7%)	21 56

All (228) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	31	VAL
1	A	36	THR
1	A	45	LEU
1	A	46	VAL
1	A	51	LYS
1	A	54	LEU
1	A	64	VAL
1	A	71	ASN
1	A	93	GLN
1	A	104	GLN
1	A	163	GLN
1	A	178	ASN
1	A	208	PRO
1	A	215	GLU
1	A	223	ILE
1	A	249	VAL
1	A	259	ARG
1	A	291	ASN
1	A	293	ARG
1	A	317	VAL
1	A	372	GLU
1	A	408	GLU
1	A	425	SER
1	A	466	ARG
1	A	475	LYS
1	A	477	ARG
1	A	492	LEU
1	A	509	LEU
1	A	521	GLN
1	A	547	GLN
1	A	551	ARG
1	A	552	GLN
1	A	596	ASP
1	A	611	LYS
1	A	639	GLN

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Mol	Chain	Res	Type
1	A	642	GLN
2	B	730	ASP
2	B	743	SER
2	B	758	GLU
2	B	783	LEU
2	B	790	LYS
2	B	813	LEU
2	B	826	ARG
2	B	834	GLN
2	B	835	ASN
2	B	841	ARG
2	B	883	THR
2	B	890	VAL
2	B	912	GLU
2	B	914	ILE
2	B	917	ASN
2	B	938	GLU
2	B	939	ASP
2	B	957	ARG
2	B	1076	GLN
2	B	1099	ASP
2	B	1106	GLU
2	B	1194	ASP
2	B	1269	GLU
2	B	1298	ARG
2	B	1332	ASP
2	B	1334	LEU
2	B	1360	ASN
2	B	1369	ARG
2	B	1375	ASP
2	B	1378	MET
2	B	1387	THR
2	B	1393	THR
2	B	1428	LYS
2	B	1431	HIS
2	B	1450	ILE
2	B	1462	ASN
2	B	1469	ARG
2	B	1477	ASP
2	B	1479	LYS
2	B	1490	ARG
2	B	1500	LYS

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Mol	Chain	Res	Type
2	B	1504	LYS
2	B	1537	ASP
2	B	1566	ILE
2	B	1567	LYS
2	B	1575	GLU
2	B	1590	TRP
2	B	1606	VAL
2	B	1618	GLU
2	B	1620	ASN
1	C	31	VAL
1	C	44	LYS
1	C	142	MET
1	C	234	THR
1	C	277	GLU
1	C	293	ARG
1	C	317	VAL
1	C	321	ARG
1	C	350	LEU
1	C	399	SER
1	C	417	ARG
1	C	437	SER
1	C	444	ARG
1	C	457	MET
1	C	464	LYS
1	C	477	ARG
1	C	509	LEU
1	C	558	GLN
1	C	625	THR
1	C	628	SER
1	C	634	GLN
1	C	639	GLN
2	D	752	ASN
2	D	789	ASP
2	D	804	MET
2	D	833	ARG
2	D	861	GLN
2	D	890	VAL
2	D	968	MET
2	D	1018	GLU
2	D	1024	LEU
2	D	1050	ARG
2	D	1141	ASN

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Mol	Chain	Res	Type
2	D	1149	LYS
2	D	1181	LYS
2	D	1186	ASN
2	D	1204	GLN
2	D	1273	ASP
2	D	1288	ARG
2	D	1298	ARG
2	D	1325	MET
2	D	1346	LYS
2	D	1369	ARG
2	D	1375	ASP
2	D	1378	MET
2	D	1393	THR
2	D	1395	ASP
2	D	1412	LEU
2	D	1428	LYS
2	D	1445	PHE
2	D	1450	ILE
2	D	1462	ASN
2	D	1469	ARG
2	D	1487	GLU
2	D	1488	LEU
2	D	1490	ARG
2	D	1499	GLN
2	D	1503	ASP
2	D	1504	LYS
2	D	1506	THR
2	D	1507	LEU
2	D	1509	GLU
2	D	1566	ILE
2	D	1567	LYS
2	D	1583	TRP
2	D	1593	LYS
2	D	1605	TRP
2	D	1625	GLN
2	D	1641	ASN
3	E	1	ASP
3	E	3	GLN
3	E	31	THR
3	E	39	LYS
3	E	63	SER
3	E	70	ASP

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Mol	Chain	Res	Type
3	E	88	CYS
3	E	89	GLN
3	E	90	GLN
3	E	94	THR
3	E	99	GLU
3	E	100	GLN
3	E	103	LYS
3	E	108	ARG
3	E	158	ASN
3	E	164	THR
3	E	187	GLU
4	F	11	LEU
4	F	12	VAL
4	F	18	LEU
4	F	32	SER
4	F	63	VAL
4	F	75	LYS
4	F	100	SER
4	F	105	GLN
4	F	107	THR
4	F	108	LEU
4	F	110	THR
4	F	116	THR
4	F	140	CYS
4	F	170	LEU
4	F	183	THR
4	F	196	CYS
4	F	208	ASP
3	G	3	GLN
3	G	12	SER
3	G	18	ARG
3	G	20	THR
3	G	23	CYS
3	G	31	THR
3	G	39	LYS
3	G	45	LYS
3	G	73	LEU
3	G	88	CYS
3	G	89	GLN
3	G	90	GLN
3	G	91	SER
3	G	108	ARG

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Mol	Chain	Res	Type
3	G	125	LEU
3	G	135	LEU
3	G	145	LYS
3	G	149	LYS
3	G	158	ASN
3	G	164	THR
3	G	165	GLU
3	G	176	SER
3	G	201	LEU
4	H	1	GLU
4	H	7	SER
4	H	12	VAL
4	H	18	LEU
4	H	28	SER
4	H	63	VAL
4	H	72	ASN
4	H	82(B)	SER
4	H	100(F)	MET
4	H	105	GLN
4	H	110	THR
4	H	160	THR
4	H	170	LEU
4	H	172	SER
4	H	189	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	28	GLN
1	A	81	ASN
1	A	162	ASN
1	A	163	GLN
1	A	178	ASN
1	A	376	GLN
1	A	395	GLN
1	A	452	ASN
1	A	490	GLN
1	A	547	GLN
1	A	558	GLN
1	A	634	GLN
2	B	836	GLN

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Mol	Chain	Res	Type
2	B	961	GLN
2	B	1069	ASN
2	B	1113	ASN
2	B	1115	ASN
2	B	1130	GLN
2	B	1141	ASN
2	B	1160	ASN
2	B	1204	GLN
2	B	1277	GLN
2	B	1317	GLN
2	B	1360	ASN
2	B	1401	ASN
2	B	1451	GLN
2	B	1462	ASN
2	B	1472	HIS
2	B	1499	GLN
2	B	1531	GLN
2	B	1559	GLN
2	B	1620	ASN
1	C	10	ASN
1	C	38	HIS
1	C	81	ASN
1	C	155	GLN
1	C	163	GLN
1	C	254	GLN
1	C	370	GLN
1	C	435	HIS
1	C	490	GLN
1	C	634	GLN
1	C	639	GLN
2	D	752	ASN
2	D	805	GLN
2	D	834	GLN
2	D	836	GLN
2	D	860	HIS
2	D	961	GLN
2	D	1130	GLN
2	D	1176	GLN
2	D	1186	ASN
2	D	1204	GLN
2	D	1327	HIS
2	D	1360	ASN

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Mol	Chain	Res	Type
2	D	1401	ASN
2	D	1451	GLN
2	D	1462	ASN
2	D	1481	ASN
2	D	1558	GLN
2	D	1621	GLN
3	E	3	GLN
3	E	89	GLN
3	E	124	GLN
3	E	158	ASN
4	F	76	ASN
4	F	200	HIS
3	G	3	GLN
3	G	90	GLN
3	G	137	ASN
3	G	147	GLN
3	G	158	ASN
3	G	160	GLN
4	H	54	ASN
4	H	72	ASN
4	H	164	HIS
4	H	200	HIS

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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	642/644 (99%)	-0.12	5 (0%) 87 75	3, 29, 61, 99	0
1	C	642/644 (99%)	-0.07	5 (0%) 87 75	3, 31, 64, 119	0
2	B	903/915 (98%)	1.01	205 (22%) 1 0	2, 72, 148, 165	0
2	D	903/915 (98%)	0.21	79 (8%) 13 4	2, 26, 144, 154	0
3	E	214/214 (100%)	0.05	1 (0%) 91 83	4, 24, 47, 82	0
3	G	214/214 (100%)	-0.22	0 100 100	2, 13, 43, 77	0
4	F	221/226 (97%)	-0.23	2 (0%) 85 72	2, 18, 58, 91	0
4	H	221/226 (97%)	-0.25	1 (0%) 91 83	2, 12, 36, 86	0
All	All	3960/3998 (99%)	0.21	298 (7%) 17 6	2, 29, 133, 165	0

All (298) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1300	GLU	10.8
2	B	919	THR	10.7
2	B	1202	GLY	10.6
2	B	1243	GLY	10.4
2	D	1318	GLY	9.2
2	D	925	LEU	8.9
2	B	924	THR	8.8
2	D	921	ALA	8.7
2	D	1294	ALA	8.6
2	D	946	SER	8.3
2	D	924	THR	8.0
2	D	963	THR	7.7
2	D	1320	LEU	7.6
2	D	951	ASP	7.3
2	D	1306	GLU	7.2
2	D	1295	SER	7.1

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Mol	Chain	Res	Type	RSRZ
2	B	934	GLY	7.1
2	B	1321	SER	7.0
2	B	937	LYS	7.0
2	B	944	ASP	6.9
2	D	933	GLU	6.8
2	D	966	ALA	6.8
2	B	1274	VAL	6.7
2	B	1324	THR	6.7
2	B	946	SER	6.7
2	B	1265	PRO	6.5
2	B	942	PRO	6.0
2	D	935	VAL	6.0
2	D	1311	THR	6.0
2	B	964	PRO	6.0
2	B	1332	ASP	5.7
2	B	1289	ILE	5.7
2	B	1317	GLN	5.7
2	B	1268	GLN	5.6
2	D	964	PRO	5.4
2	D	1280	SER	5.4
2	B	933	GLU	5.3
2	B	1272	LEU	5.3
2	D	922	VAL	5.3
2	B	1287	HIS	5.3
2	B	1320	LEU	5.2
2	B	1273	ASP	5.2
2	B	932	ARG	5.2
2	B	1267	HIS	5.1
2	D	1307	GLY	5.1
2	D	926	ASP	5.1
2	B	943	ALA	5.0
2	B	1040	PRO	5.0
2	D	1322	VAL	5.0
2	B	929	ARG	4.9
2	B	1238	ARG	4.9
2	B	1073	ILE	4.9
2	B	1049	LYS	4.9
2	B	1099	ASP	4.8
2	B	1279	PRO	4.8
2	B	1115	ASN	4.8
2	B	1266	ASP	4.8
2	B	1263	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	920	VAL	4.7
2	D	1310	VAL	4.7
2	B	1047	PHE	4.6
2	B	1318	GLY	4.7
2	B	1069	ASN	4.6
2	B	963	THR	4.6
2	D	1313	GLU	4.6
2	B	918	LYS	4.6
1	A	48	SER	4.5
1	C	48	SER	4.5
2	B	968	MET	4.5
2	D	1276	LEU	4.5
2	B	1196	ASN	4.5
2	B	958	ILE	4.5
2	B	1282	SER	4.5
2	B	1038	ARG	4.5
2	D	1332	ASP	4.5
2	B	1319	THR	4.5
2	D	1285	ILE	4.4
2	D	919	THR	4.4
2	B	1183	PRO	4.4
2	D	1319	THR	4.3
2	B	1322	VAL	4.3
2	D	1317	GLN	4.3
2	B	1201	PRO	4.3
2	B	956	THR	4.2
2	B	962	GLY	4.2
2	B	1311	THR	4.2
2	B	1200	ASP	4.2
2	B	965	VAL	4.2
1	A	76	SER	4.2
2	B	947	ASP	4.2
2	B	1157	ASN	4.2
2	D	1312	ALA	4.1
2	B	1264	ALA	4.1
2	B	1142	SER	4.1
2	D	1304	GLU	4.1
2	B	1307	GLY	4.1
2	B	939	ASP	4.1
2	B	1048	VAL	4.1
2	B	938	GLU	4.1
2	B	930	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	1160	ASN	4.0
2	B	1204	GLN	4.0
2	D	920	VAL	3.9
2	D	1316	GLY	3.9
2	B	941	PRO	3.9
2	B	1290	HIS	3.9
2	B	966	ALA	3.9
2	B	1276	LEU	3.9
2	B	923	ARG	3.9
2	B	1053	SER	3.9
2	B	1242	GLY	3.9
2	B	1092	PRO	3.8
2	B	957	ARG	3.8
2	B	935	VAL	3.8
2	D	932	ARG	3.8
2	D	936	GLN	3.8
2	B	954	SER	3.8
2	B	960	LEU	3.7
2	D	1270	LEU	3.7
2	B	1194	ASP	3.7
2	B	1177	MET	3.7
2	B	1134	ASP	3.7
2	B	1235	ASN	3.7
2	B	1306	GLU	3.7
2	D	961	GLN	3.6
2	B	1277	GLN	3.6
2	B	931	GLY	3.6
1	C	76	SER	3.6
2	B	1101	PRO	3.6
2	B	936	GLN	3.6
2	B	1154	LEU	3.6
2	B	925	LEU	3.5
2	B	1221	LEU	3.5
2	D	1297	LEU	3.5
2	D	1303	LYS	3.5
2	B	1162	GLN	3.5
2	B	1025	GLU	3.5
2	B	1184	LEU	3.4
2	D	940	ILE	3.4
2	D	1309	THR	3.4
2	B	1197	ARG	3.4
2	D	950	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	958	ILE	3.4
2	B	1036	ALA	3.4
2	B	1158	TYR	3.3
2	B	1310	VAL	3.3
2	D	918	LYS	3.2
2	B	1138	GLU	3.2
2	B	1351	THR	3.2
2	D	1289	ILE	3.2
2	B	921	ALA	3.2
2	D	965	VAL	3.1
2	B	1141	ASN	3.1
2	B	1180	LEU	3.1
2	D	1302	THR	3.1
2	B	1096	PHE	3.1
2	B	1074	ASP	3.1
2	B	976	GLU	3.1
2	B	1203	LYS	3.1
2	B	928	GLU	3.1
2	B	1326	TYR	3.0
2	B	1325	MET	3.0
2	B	1191	THR	3.0
2	D	1287	HIS	3.0
2	D	1329	LYS	3.0
2	B	926	ASP	3.0
2	B	1244	TYR	3.0
2	D	937	LYS	3.0
2	B	959	LEU	3.0
2	B	1199	GLU	3.0
1	A	371	GLY	3.0
2	B	1075	SER	2.9
2	B	1024	LEU	2.9
2	B	1198	TRP	2.9
2	B	1094	GLY	2.9
2	B	1305	ASN	2.9
2	B	1333	GLN	2.9
2	B	1093	ASP	2.9
2	B	927	PRO	2.9
2	B	948	GLN	2.9
2	D	1293	SER	2.9
2	B	961	GLN	2.9
2	D	923	ARG	2.9
2	D	1284	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	1308	PHE	2.8
2	B	1137	GLU	2.8
2	B	1286	THR	2.8
2	B	1193	LYS	2.8
2	B	1299	SER	2.8
2	D	960	LEU	2.8
2	D	1272	LEU	2.8
2	B	1284	LYS	2.8
2	B	1275	SER	2.8
2	D	945	LEU	2.8
2	D	1351	THR	2.8
2	D	962	GLY	2.8
1	C	374	THR	2.8
2	D	1279	PRO	2.8
2	B	1039	GLN	2.8
2	B	971	ASP	2.7
2	B	1091	LYS	2.7
4	F	216	CYS	2.7
2	B	1168	ALA	2.7
2	B	1088	GLU	2.7
2	B	1540	ILE	2.7
2	B	1133	LYS	2.6
2	D	1305	ASN	2.6
2	B	1298	ARG	2.6
2	D	1269	GLU	2.6
2	D	934	GLY	2.6
2	B	1500	LYS	2.6
2	B	1283	SER	2.6
2	D	939	ASP	2.6
2	B	1297	LEU	2.6
2	B	1295	SER	2.6
2	B	1232	ARG	2.6
1	C	71	ASN	2.6
2	B	1116	GLU	2.6
2	B	1174	LEU	2.6
2	B	1350	GLU	2.6
2	D	1301	GLU	2.6
2	B	1271	ASN	2.5
2	B	1072	ALA	2.5
2	B	1240	TYR	2.5
2	B	1050	ARG	2.5
2	B	1044	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	1206	TYR	2.5
2	B	1104	HIS	2.5
2	B	1114	ASN	2.5
2	B	1359	LYS	2.5
2	D	1278	LEU	2.4
2	D	1267	HIS	2.4
2	B	1136	CYS	2.4
2	B	970	GLU	2.4
2	B	1035	LEU	2.4
4	F	214	LYS	2.4
2	B	1534	ASN	2.4
2	B	1018	GLU	2.4
2	B	1188	PHE	2.4
2	B	1288	ARG	2.4
2	B	1313	GLU	2.3
2	D	1350	GLU	2.3
2	B	1349	PRO	2.3
2	B	1146	SER	2.3
2	B	1302	THR	2.3
2	B	1192	ALA	2.3
2	B	1205	LEU	2.3
2	B	1190	THR	2.3
2	B	1296	LEU	2.3
3	E	134	CYS	2.3
2	B	1052	PRO	2.3
2	D	1594	PRO	2.3
2	B	1292	GLU	2.3
2	B	1076	GLN	2.3
2	D	1333	GLN	2.2
1	A	374	THR	2.2
2	B	945	LEU	2.2
2	B	1312	ALA	2.2
2	B	1323	VAL	2.2
2	B	1173	ALA	2.2
2	B	1117	LYS	2.2
2	B	1531	GLN	2.2
2	D	1321	SER	2.2
2	B	1309	THR	2.2
2	D	1114	ASN	2.2
1	A	30	ASP	2.2
2	B	1084	TRP	2.2
2	B	922	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	1042	SER	2.2
2	B	1100	ALA	2.2
2	B	1256	ALA	2.2
2	D	1300	GLU	2.2
2	B	1089	LYS	2.2
2	B	1150	ALA	2.2
2	B	1278	LEU	2.2
2	B	973	VAL	2.2
2	D	1273	ASP	2.1
2	D	1266	ASP	2.1
2	B	988	CYS	2.1
2	D	930	LEU	2.1
2	B	1281	ARG	2.1
2	B	1181	LYS	2.1
2	D	1416	PHE	2.1
2	B	1314	GLY	2.1
2	B	1032	THR	2.1
2	B	1294	ALA	2.1
4	H	216	CYS	2.1
2	B	1212	SER	2.1
2	D	941	PRO	2.1
2	B	1241	GLY	2.1
2	B	967	GLN	2.1
2	B	1224	PHE	2.0
2	D	1314	GLY	2.0
2	B	1593	LYS	2.0
1	C	521	GLN	2.0
2	B	1135	ILE	2.0
2	B	1270	LEU	2.0
2	B	1316	GLY	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

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
5	CA	A	645	1/1	0.92	0.13	-1.29	47,47,47,47	0
5	CA	C	645	1/1	0.94	0.13	-1.65	54,54,54,54	0

6.5 Other polymers

There are no such residues in this entry.