Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 09:04 PM GMT

PDB ID	:	4XPI
Title	:	Fe protein independent substrate reduction by nitrogenase variants altered in intramolecular electron transfer
Authors	:	Danyal, K.; Rasmusen, A.J.; Keable, S.M.; Shaw, S.; Zadvornyy, O.; Duval, S.; Dean, D.R.; Raugei, S.; Peters, J.W.; Seefeldt, L.C.
Deposited on	:	2015-01-17
Resolution	:	1.97 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:

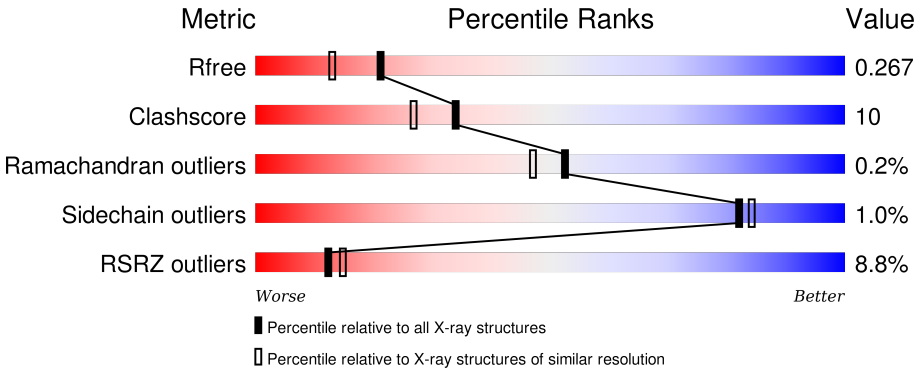
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 1.97 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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	490	11% 79% 18%
1	C	490	16% 71% 25%
2	B	522	4% 86% 13%
2	D	522	4% 87% 13%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	B	606	-	-	-	X
5	GOL	B	607	-	-	X	X
5	GOL	B	608	-	-	X	X
5	GOL	C	505	-	-	X	X
5	GOL	C	506	-	-	-	X
5	GOL	C	508	-	-	X	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 17075 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 Nitrogenase molybdenum-iron protein alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	1	2	0
			3805	2419	648	712	26			
1	C	478	Total	C	N	O	S	0	1	0
			3797	2414	647	711	25			

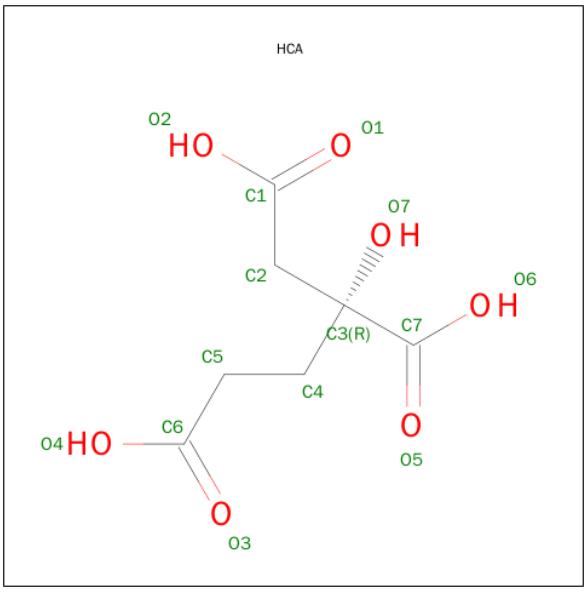
- Molecule 2 is a protein called Nitrogenase molybdenum-iron protein beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	1	0
			4178	2666	708	776	28			
2	D	522	Total	C	N	O	S	0	0	0
			4172	2663	707	774	28			

There are 2 discrepancies between the modelled and reference sequences:

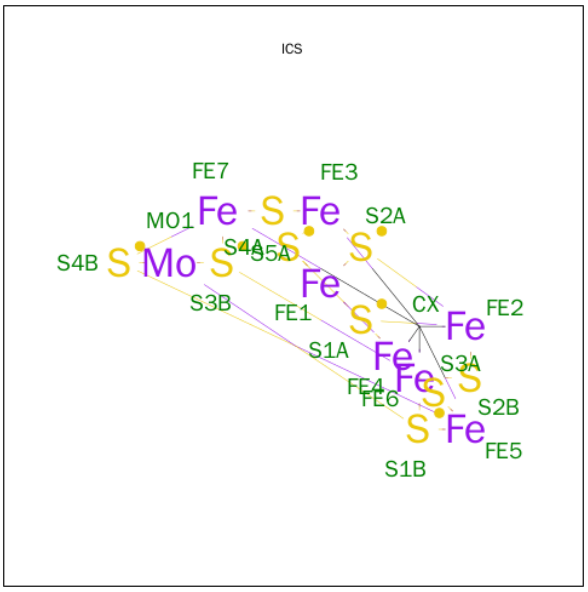
Chain	Residue	Modelled	Actual	Comment	Reference
B	98	HIS	TYR	engineered mutation	UNP P07329
D	98	HIS	TYR	engineered mutation	UNP P07329

- Molecule 3 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: $C_7H_{10}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 14 7 7	0	0
3	C	1	Total C O 14 7 7	0	0

- Molecule 4 is iron-sulfur-molybdenum cluster with interstitial carbon (three-letter code: ICS) (formula: CFe_7MoS_9).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Fe Mo S 18 1 7 1 9	0	0

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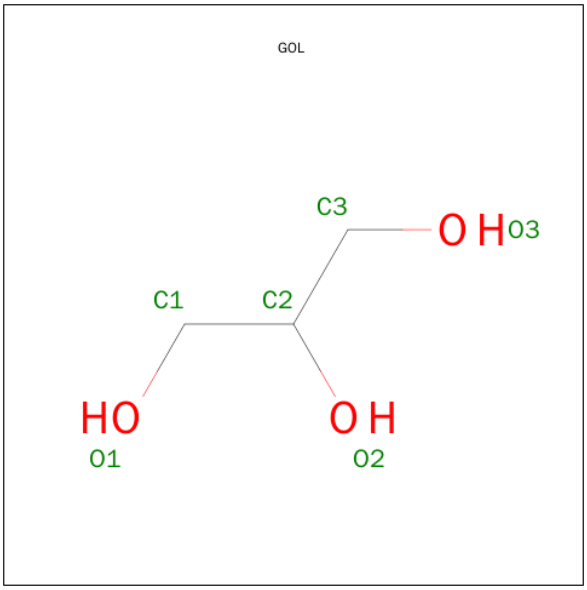
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	Fe	Mo	S	0	0
			18	1	7	1	9		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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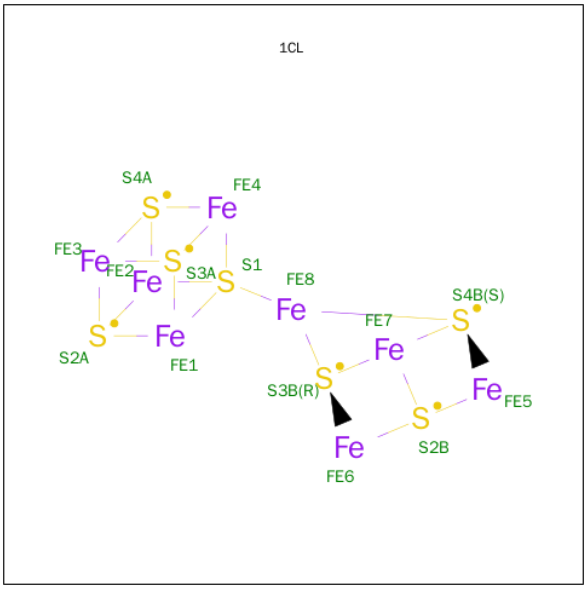
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

- Molecule 6 is FE(8)-S(7) CLUSTER, OXIDIZED (three-letter code: 1CL) (formula: Fe_8S_7).



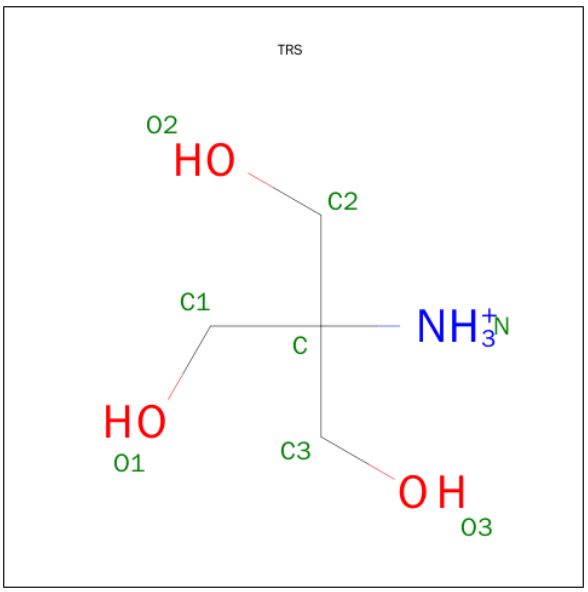
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Fe S 15 8 7	0	0
6	C	1	Total Fe S 15 8 7	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	2	Total Ca 2 2	0	0

- Molecule 8 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code:

TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O 8 4 1 3	0	0
8	D	1	Total C N O 8 4 1 3	0	0

- Molecule 9 is water.

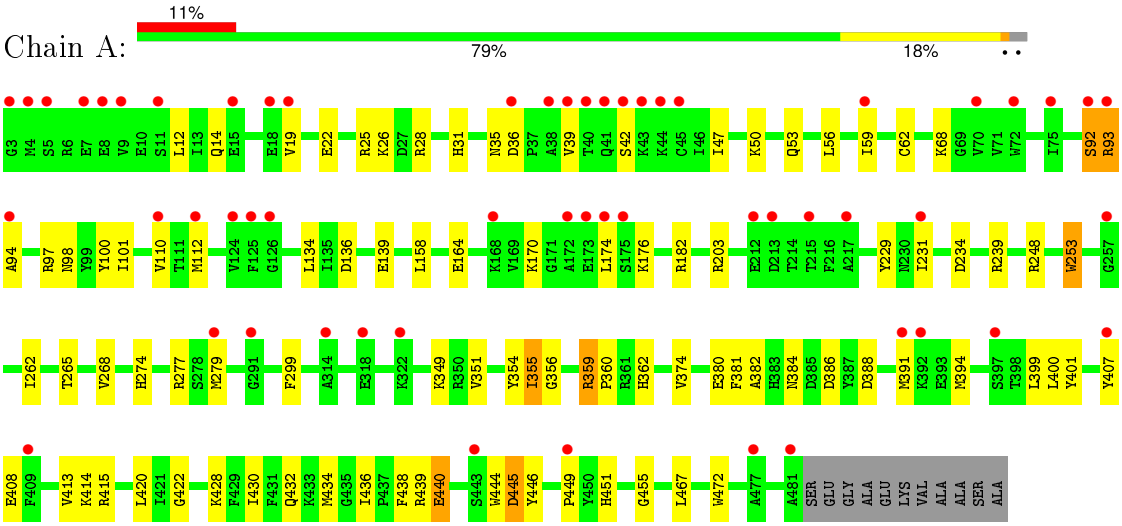
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	211	Total O 211 211	0	0
9	B	257	Total O 257 257	0	0
9	C	202	Total O 202 202	0	0
9	D	251	Total O 251 251	0	0

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.

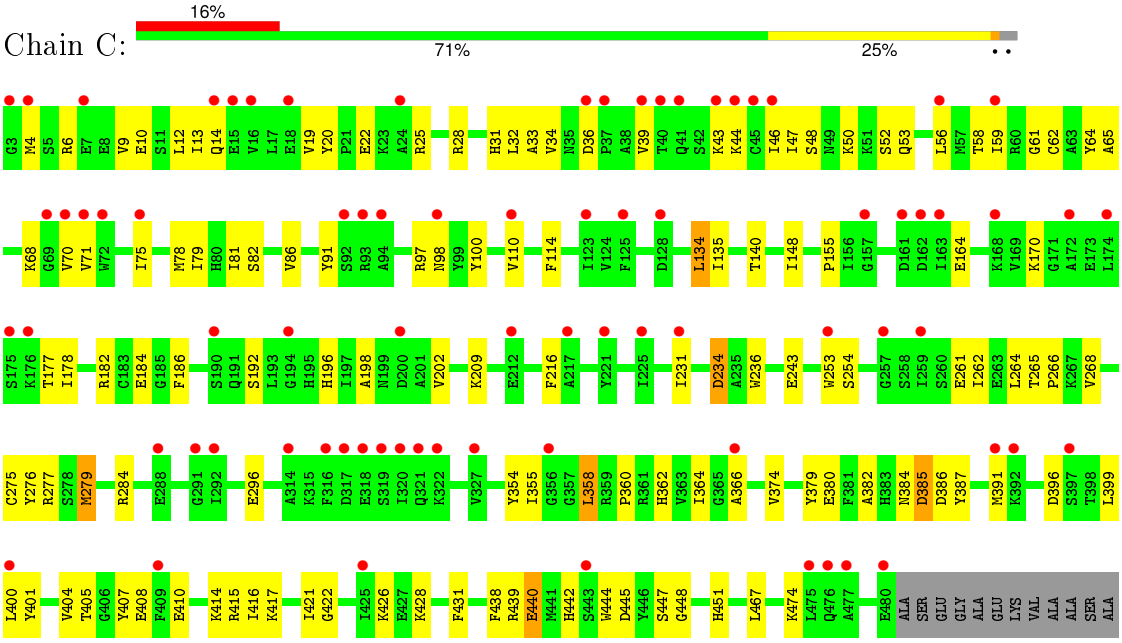
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

Chain A:



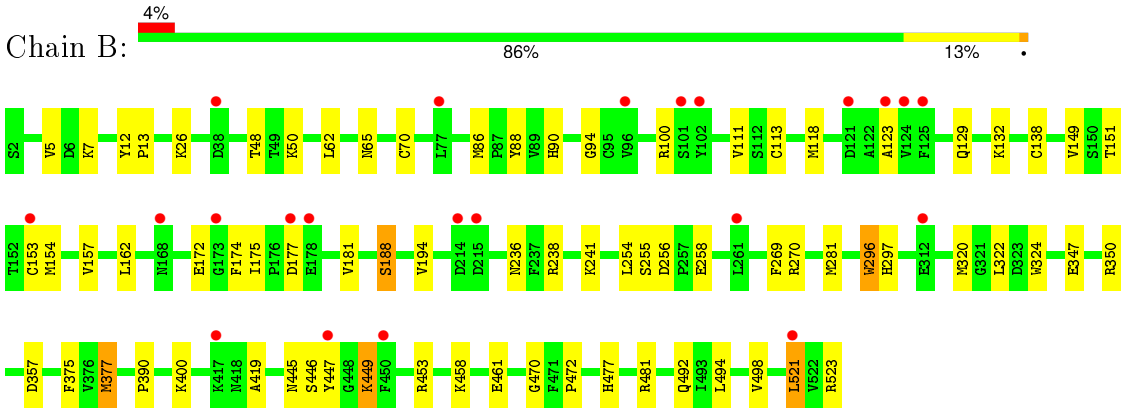
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

Chain C:



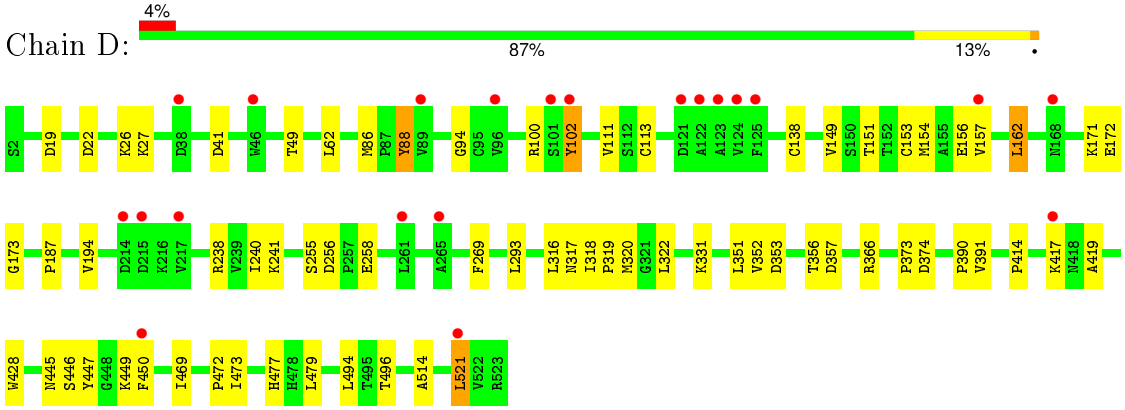
- Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain B:



- Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.80Å 130.83Å 108.11Å 90.00° 111.14° 90.00°	Depositor
Resolution (Å)	35.00 – 1.97 35.89 – 1.97	Depositor EDS
% Data completeness (in resolution range)	96.4 (35.00-1.97) 96.4 (35.89-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.213 , 0.264 0.218 , 0.267	Depositor DCC
R_{free} test set	7091 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	27.7	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 49.0	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 141514 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17075	wwPDB-VP
Average B, all atoms (Å^2)	41.0	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 24.75 % 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 3.6143e-03.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, 0.375 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: GOL, CA, HCA, ICS, TRS, 1CL

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	1.06	7/3899 (0.2%)	0.96	6/5257 (0.1%)
1	C	0.93	4/3888 (0.1%)	0.92	4/5242 (0.1%)
2	B	1.03	6/4284 (0.1%)	0.94	7/5791 (0.1%)
2	D	1.01	6/4278 (0.1%)	0.92	8/5783 (0.1%)
All	All	1.01	23/16349 (0.1%)	0.94	25/22073 (0.1%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	440	GLU	CD-OE2	-11.81	1.12	1.25
1	A	92	SER	CA-C	-11.61	1.22	1.52
1	C	440	GLU	CD-OE2	-8.55	1.16	1.25
2	B	357	ASP	C-O	7.68	1.38	1.23
1	C	91	TYR	CD1-CE1	-7.25	1.28	1.39
2	D	428	TRP	CD2-CE2	7.22	1.50	1.41
2	D	357	ASP	C-O	7.02	1.36	1.23
1	A	430	ILE	C-O	6.86	1.36	1.23
1	A	356	GLY	C-O	-6.78	1.12	1.23
2	B	188	SER	CB-OG	6.52	1.50	1.42
2	D	450	PHE	N-CA	6.23	1.58	1.46
2	D	477	HIS	CG-CD2	6.20	1.46	1.35
1	C	444	TRP	CD2-CE2	6.17	1.48	1.41
2	B	324	TRP	CD2-CE2	5.86	1.48	1.41
1	A	444	TRP	CD2-CE2	5.86	1.48	1.41
2	B	477	HIS	CG-CD2	5.68	1.45	1.35
2	D	102	TYR	CE2-CZ	-5.62	1.31	1.38
1	A	229	TYR	CG-CD2	5.48	1.46	1.39
2	D	496	THR	C-O	5.39	1.33	1.23
1	C	236	TRP	CD2-CE2	5.36	1.47	1.41
2	B	477	HIS	CE1-NE2	5.26	1.44	1.32
1	A	253	TRP	CG-CD1	5.12	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	296	TRP	CD2-CE2	5.00	1.47	1.41

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	320	MET	CG-SD-CE	7.86	112.78	100.20
2	D	521	LEU	CB-CG-CD2	7.45	123.66	111.00
1	A	93	ARG	NE-CZ-NH2	-6.94	116.83	120.30
2	B	521	LEU	CB-CG-CD2	6.89	122.72	111.00
2	B	377	MET	CG-SD-CE	-6.65	89.56	100.20
1	C	134	LEU	CB-CG-CD1	-6.21	100.45	111.00
1	C	234	ASP	CB-CG-OD1	6.11	123.80	118.30
1	C	358	LEU	CB-CG-CD2	-6.08	100.66	111.00
2	D	41	ASP	CB-CG-OD1	5.99	123.69	118.30
2	B	481	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	203	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	359	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	239	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	C	385	ASP	CB-CG-OD1	5.59	123.33	118.30
2	D	238	ARG	NE-CZ-NH2	-5.50	117.55	120.30
2	B	498	VAL	CG1-CB-CG2	-5.50	102.10	110.90
2	D	162	LEU	CB-CG-CD1	-5.31	101.97	111.00
2	D	469	ILE	CG1-CB-CG2	-5.29	99.75	111.40
2	D	19	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	445	ASP	CB-CG-OD1	5.23	123.01	118.30
2	B	238	ARG	NE-CZ-NH2	-5.09	117.75	120.30
2	B	350	ARG	NE-CZ-NH2	-5.05	117.78	120.30
2	B	523	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	A	248	ARG	NE-CZ-NH2	-5.05	117.78	120.30
2	D	374	ASP	CB-CG-OD1	5.03	122.82	118.30

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	3805	0	3747	83	0
1	C	3797	0	3737	135	0
2	B	4178	0	4089	63	0
2	D	4172	0	4085	45	0
3	A	14	0	6	1	0
3	C	14	0	6	2	0
4	A	18	0	0	0	0
4	C	18	0	0	0	0
5	A	6	0	8	0	0
5	B	36	0	48	17	0
5	C	36	0	48	19	0
5	D	12	0	16	0	0
6	A	15	0	0	0	0
6	C	15	0	0	0	0
7	B	2	0	0	0	0
8	B	8	0	12	2	0
8	D	8	0	12	1	0
9	A	211	0	0	22	0
9	B	257	0	0	25	0
9	C	202	0	0	52	0
9	D	251	0	0	16	0
All	All	17075	0	15814	324	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 10.

All (324) 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:C:71:VAL:HG13	9:C:796:HOH:O	1.24	1.35
1:C:428:LYS:HB2	9:C:766:HOH:O	1.39	1.17
1:C:385:ASP:HB2	9:C:691:HOH:O	1.38	1.17
1:C:358:LEU:HB2	9:C:615:HOH:O	1.61	0.99
1:C:46:ILE:HD12	9:C:730:HOH:O	1.60	0.98
2:B:111:VAL:HG12	9:B:735:HOH:O	1.67	0.95
5:C:504:GOL:O3	9:C:601:HOH:O	1.81	0.93
1:C:428:LYS:HD2	9:C:609:HOH:O	1.69	0.91
1:C:36:ASP:O	1:C:39:VAL:HG22	1.69	0.91
2:D:318:ILE:HA	9:D:701:HOH:O	1.69	0.91
1:A:394:MET:HB2	9:A:719:HOH:O	1.72	0.90
2:D:111:VAL:HG12	9:D:727:HOH:O	1.72	0.89
2:B:269:PHE:CD2	9:B:819:HOH:O	2.26	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:269:PHE:CD2	9:D:871:HOH:O	2.27	0.88
1:C:438:PHE:HB2	9:C:667:HOH:O	1.75	0.87
1:C:25:ARG:NH1	9:C:602:HOH:O	2.08	0.86
5:C:504:GOL:C3	9:C:601:HOH:O	2.23	0.86
1:C:140:THR:HG21	5:C:507:GOL:H12	1.55	0.86
2:D:194:VAL:HG21	9:D:925:HOH:O	1.76	0.85
1:A:440:GLU:HG3	9:A:785:HOH:O	1.75	0.85
1:A:428:LYS:HB2	9:A:785:HOH:O	1.76	0.84
1:C:6:ARG:NH2	1:C:396:ASP:OD1	2.11	0.83
1:C:28:ARG:HD3	1:C:408:GLU:OE2	1.79	0.82
1:A:36:ASP:O	1:A:39:VAL:HG22	1.80	0.82
1:C:186:PHE:HB3	9:D:773:HOH:O	1.78	0.81
1:A:445:ASP:OD2	9:A:601:HOH:O	2.00	0.80
1:C:13:ILE:HG21	9:C:741:HOH:O	1.81	0.79
1:C:416:ILE:HG13	9:C:737:HOH:O	1.82	0.79
2:B:90:HIS:HB2	9:B:801:HOH:O	1.82	0.78
2:D:100:ARG:HG3	9:D:932:HOH:O	1.84	0.78
1:A:440:GLU:CG	9:A:785:HOH:O	2.27	0.78
2:B:461:GLU:OE1	9:B:701:HOH:O	2.01	0.77
1:A:139:GLU:HG3	1:A:174:LEU:HD13	1.69	0.75
1:C:78:MET:HE2	9:C:628:HOH:O	1.87	0.75
1:A:432:GLN:OE1	9:A:602:HOH:O	2.05	0.74
2:D:293:LEU:O	9:D:701:HOH:O	2.03	0.74
2:B:88:TYR:HE2	9:B:801:HOH:O	1.70	0.74
1:C:61:GLY:HA3	9:C:656:HOH:O	1.86	0.74
1:C:234:ASP:HB3	1:C:451:HIS:ND1	2.03	0.74
1:C:58:THR:HB	5:C:508:GOL:O1	1.89	0.72
1:C:64:TYR:HB2	9:C:627:HOH:O	1.88	0.72
1:C:253:TRP:HB3	1:C:279:MET:CE	2.20	0.72
1:C:385:ASP:CB	9:C:691:HOH:O	2.14	0.72
1:A:253:TRP:HB3	1:A:279:MET:HE1	1.72	0.70
2:B:129:GLN:HA	9:B:718:HOH:O	1.90	0.70
1:C:410:GLU:OE2	1:C:414:LYS:NZ	2.23	0.69
1:A:42:SER:N	1:A:388:ASP:OD1	2.19	0.69
1:A:53:GLN:HB2	1:A:56:LEU:HD12	1.73	0.69
5:C:504:GOL:H31	9:C:601:HOH:O	1.91	0.69
1:C:275:CYS:HB2	9:C:765:HOH:O	1.93	0.68
2:B:347:GLU:OE2	9:B:702:HOH:O	2.12	0.67
1:C:12:LEU:HD13	1:C:415:ARG:HG2	1.76	0.66
1:C:4:MET:SD	9:C:737:HOH:O	2.54	0.66
1:A:351:VAL:CG2	1:A:374:VAL:HG22	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:373:PRO:HD2	9:D:925:HOH:O	1.96	0.66
1:A:445:ASP:CG	9:A:601:HOH:O	2.34	0.66
1:A:428:LYS:NZ	9:A:605:HOH:O	2.28	0.66
1:C:467:LEU:O	1:C:467:LEU:HD23	1.96	0.66
1:C:28:ARG:CD	1:C:408:GLU:OE2	2.42	0.65
1:C:33:ALA:HB3	9:C:730:HOH:O	1.97	0.65
1:C:53:GLN:HB2	1:C:56:LEU:HD12	1.79	0.65
1:C:209:LYS:HE2	9:C:659:HOH:O	1.97	0.64
2:B:236:ASN:ND2	5:B:607:GOL:H12	2.13	0.64
1:C:10:GLU:HG3	1:C:34:VAL:HG21	1.79	0.64
1:A:93:ARG:NH2	5:B:608:GOL:O2	2.31	0.64
2:B:129:GLN:OE1	9:B:703:HOH:O	2.15	0.63
1:A:101:ILE:HD12	5:B:603:GOL:H31	1.80	0.63
1:C:416:ILE:CG1	9:C:737:HOH:O	2.42	0.63
2:D:353:ASP:OD2	9:D:702:HOH:O	2.16	0.63
1:A:62:CYS:HA	9:A:641:HOH:O	1.98	0.62
1:C:32:LEU:HD21	9:C:753:HOH:O	1.98	0.62
1:A:391:MET:HA	9:A:719:HOH:O	2.00	0.62
1:A:35:ASN:HB2	1:A:400:LEU:HD11	1.82	0.62
1:C:192:SER:OG	9:C:603:HOH:O	2.16	0.62
1:C:253:TRP:HB3	1:C:279:MET:HE1	1.82	0.61
1:A:134:LEU:HG	2:B:62:LEU:HB2	1.82	0.61
1:C:71:VAL:CG1	9:C:796:HOH:O	2.04	0.61
1:C:53:GLN:O	5:C:508:GOL:C1	2.49	0.61
1:C:440:GLU:HG3	9:C:766:HOH:O	2.00	0.60
1:C:53:GLN:N	5:C:508:GOL:H11	2.16	0.60
1:C:14:GLN:HB3	9:C:764:HOH:O	2.01	0.60
1:C:400:LEU:CB	9:C:730:HOH:O	2.49	0.60
1:C:253:TRP:HB3	1:C:279:MET:HE3	1.82	0.60
2:B:7:LYS:HD3	9:B:810:HOH:O	2.02	0.59
2:B:446:SER:O	2:B:449:LYS:HG2	2.02	0.59
2:B:65:ASN:HD21	5:B:608:GOL:H31	1.67	0.58
9:C:604:HOH:O	2:D:26:LYS:HB2	2.04	0.58
1:C:47:ILE:CD1	1:C:50:LYS:HG3	2.34	0.58
2:B:172:GLU:OE1	9:B:704:HOH:O	2.17	0.58
1:C:438:PHE:CB	9:C:667:HOH:O	2.41	0.58
2:D:366:ARG:NH2	2:D:391:VAL:HG21	2.18	0.57
1:C:400:LEU:HB3	9:C:730:HOH:O	2.03	0.57
1:C:254:SER:HB3	9:C:748:HOH:O	2.04	0.57
1:C:81:ILE:C	9:C:630:HOH:O	2.43	0.57
1:C:47:ILE:HD12	1:C:50:LYS:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:MET:HG2	5:B:608:GOL:O2	2.05	0.57
1:A:39:VAL:HG23	1:A:39:VAL:O	2.05	0.56
1:A:445:ASP:O	1:A:446:TYR:HB2	2.05	0.56
2:B:90:HIS:CE1	2:B:118:MET:SD	2.99	0.56
1:C:405:THR:HG22	5:C:508:GOL:O3	2.05	0.56
1:C:216:PHE:CD1	1:C:264:LEU:HD22	2.41	0.56
2:B:100:ARG:HG3	9:B:947:HOH:O	2.04	0.56
1:A:47:ILE:HD12	1:A:50:LYS:HG2	1.89	0.55
1:C:48:SER:OG	1:C:384:ASN:ND2	2.38	0.55
2:D:390:PRO:O	2:D:419:ALA:HB2	2.06	0.55
1:C:39:VAL:O	1:C:39:VAL:HG23	2.07	0.55
1:A:164:GLU:OE1	1:A:182:ARG:NH2	2.41	0.54
2:D:113:CYS:HB2	9:D:727:HOH:O	2.06	0.54
1:C:467:LEU:C	1:C:467:LEU:HD23	2.28	0.54
1:C:265:THR:O	1:C:268:VAL:HG22	2.06	0.54
1:A:22:GLU:HG3	1:A:25:ARG:NH2	2.23	0.54
1:C:68:LYS:HD3	1:C:68:LYS:C	2.28	0.54
1:A:354:TYR:OH	1:A:380:GLU:HA	2.08	0.54
2:B:151:THR:HG23	2:B:162:LEU:HD11	1.89	0.54
1:C:164:GLU:OE1	1:C:182:ARG:NH2	2.40	0.54
1:C:44:LYS:NZ	9:C:614:HOH:O	2.39	0.53
1:C:65:ALA:O	1:C:70:VAL:HG23	2.08	0.53
1:C:53:GLN:O	5:C:508:GOL:H12	2.08	0.53
1:C:59:ILE:HD12	1:C:354:TYR:CE2	2.43	0.53
1:A:440:GLU:HG3	9:A:601:HOH:O	2.08	0.53
1:C:110:VAL:O	5:C:505:GOL:H11	2.08	0.53
1:A:164:GLU:OE2	1:A:182:ARG:NE	2.41	0.53
2:B:7:LYS:HE2	9:B:946:HOH:O	2.09	0.53
1:A:28:ARG:HD3	1:A:408:GLU:OE2	2.08	0.53
1:A:139:GLU:OE2	1:A:176:LYS:HE2	2.10	0.52
1:A:384:ASN:ND2	9:A:607:HOH:O	2.40	0.52
1:A:349:LYS:HE2	9:A:630:HOH:O	2.09	0.52
1:A:428:LYS:HD2	9:A:601:HOH:O	2.10	0.52
1:C:354:TYR:OH	1:C:380:GLU:HA	2.08	0.52
1:C:198:ALA:O	1:C:202:VAL:HG23	2.09	0.52
2:D:153:CYS:O	2:D:157:VAL:HG23	2.10	0.52
1:C:428:LYS:NZ	9:C:607:HOH:O	2.28	0.52
1:C:400:LEU:HB2	9:C:730:HOH:O	2.10	0.52
1:C:177:THR:HG21	9:C:659:HOH:O	2.10	0.52
1:C:404:VAL:HG23	9:C:753:HOH:O	2.10	0.51
2:B:50:LYS:HB2	8:B:604:TRS:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:390:PRO:O	2:B:419:ALA:HB2	2.10	0.51
1:A:12:LEU:HD13	1:A:415:ARG:HG2	1.92	0.51
2:B:453:ARG:NH1	5:B:608:GOL:O1	2.43	0.51
2:D:445:ASN:HB2	2:D:472:PRO:O	2.10	0.51
1:C:253:TRP:CB	1:C:279:MET:HE3	2.39	0.51
1:C:32:LEU:CD2	9:C:753:HOH:O	2.57	0.51
1:A:14:GLN:NE2	9:A:623:HOH:O	2.43	0.51
1:C:140:THR:CG2	5:C:507:GOL:H12	2.36	0.51
1:C:355:ILE:HB	1:C:360:PRO:HD3	1.92	0.51
2:B:322:LEU:HD21	1:C:474:LYS:HB3	1.92	0.51
1:C:354:TYR:CZ	1:C:404:VAL:HG12	2.46	0.51
1:A:445:ASP:O	1:A:446:TYR:CB	2.57	0.50
1:A:432:GLN:HG2	1:A:472:TRP:HH2	1.76	0.50
1:A:274:HIS:HE1	1:A:299:PHE:H	1.58	0.50
1:C:135:ILE:HD12	1:C:170:LYS:HG3	1.92	0.50
1:A:265:THR:O	1:A:268:VAL:HG22	2.11	0.50
1:C:52:SER:HB3	5:C:508:GOL:H11	1.92	0.50
2:B:132:LYS:HD2	9:B:718:HOH:O	2.10	0.50
1:A:28:ARG:CD	1:A:408:GLU:OE2	2.60	0.50
3:C:501:HCA:O7	3:C:501:HCA:O1	2.28	0.50
2:B:445:ASN:HA	9:B:725:HOH:O	2.11	0.50
2:D:154:MET:SD	9:D:773:HOH:O	2.59	0.49
9:A:637:HOH:O	2:B:26:LYS:HB2	2.12	0.49
2:B:296:TRP:CD1	2:B:377:MET:CE	2.95	0.49
1:C:75:ILE:HD13	1:C:262:ILE:HD11	1.95	0.49
5:B:603:GOL:H2	9:B:875:HOH:O	2.12	0.49
1:C:110:VAL:O	5:C:505:GOL:C1	2.60	0.49
3:A:501:HCA:O7	3:A:501:HCA:O2	2.29	0.49
1:A:253:TRP:HB3	1:A:279:MET:CE	2.41	0.49
1:A:47:ILE:HD11	9:A:611:HOH:O	2.11	0.49
2:B:123:ALA:HB2	2:B:154:MET:CE	2.43	0.49
2:D:171:LYS:HE2	9:D:815:HOH:O	2.13	0.49
1:C:75:ILE:HD11	9:C:748:HOH:O	2.12	0.48
1:C:19:VAL:HG11	1:C:407:TYR:CZ	2.48	0.48
2:B:153:CYS:O	2:B:157:VAL:HG23	2.13	0.48
1:C:243:GLU:OE1	9:C:604:HOH:O	2.20	0.48
1:A:413:VAL:CG1	1:A:436:ILE:CD1	2.91	0.48
2:D:319:PRO:HD3	9:D:701:HOH:O	2.12	0.48
1:C:53:GLN:O	5:C:508:GOL:H11	2.12	0.48
1:A:62:CYS:HB3	2:B:94:GLY:HA3	1.93	0.48
1:A:274:HIS:CE1	1:A:299:PHE:H	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LYS:C	1:A:68:LYS:HD3	2.33	0.48
1:C:100:TYR:CE2	1:C:110:VAL:HB	2.48	0.48
2:B:132:LYS:CD	9:B:718:HOH:O	2.62	0.47
2:B:400:LYS:H	5:B:602:GOL:H32	1.79	0.47
1:C:81:ILE:HD12	1:C:134:LEU:HD21	1.96	0.47
1:A:100:TYR:CE2	1:A:110:VAL:HB	2.49	0.47
1:A:93:ARG:NH2	5:B:608:GOL:C2	2.77	0.47
2:D:473:ILE:HG21	2:D:479:LEU:HD12	1.97	0.47
1:C:442:HIS:HB3	3:C:501:HCA:O5	2.13	0.47
2:B:111:VAL:CG1	9:B:735:HOH:O	2.42	0.47
1:C:405:THR:HG22	5:C:508:GOL:C3	2.45	0.47
1:C:134:LEU:HG	2:D:62:LEU:HB2	1.97	0.47
1:A:428:LYS:HB2	1:A:438:PHE:CE2	2.50	0.47
2:B:296:TRP:CD1	2:B:377:MET:HE1	2.50	0.47
1:A:12:LEU:HD12	9:A:649:HOH:O	2.15	0.47
1:A:445:ASP:OD1	9:A:601:HOH:O	2.19	0.47
2:D:446:SER:O	2:D:449:LYS:HG2	2.14	0.47
1:C:31:HIS:NE2	1:C:47:ILE:HD11	2.30	0.47
1:A:422:GLY:HA2	1:A:439:ARG:O	2.15	0.47
1:C:79:ILE:HG23	1:C:114:PHE:CD2	2.50	0.47
2:D:173:GLY:HA2	9:D:791:HOH:O	2.14	0.46
1:A:351:VAL:HG21	1:A:374:VAL:HG22	1.97	0.46
1:C:261:GLU:CD	2:D:27:LYS:HZ3	2.19	0.46
1:C:9:VAL:CG1	1:C:34:VAL:HG22	2.45	0.46
1:A:47:ILE:HD12	1:A:50:LYS:CG	2.45	0.46
1:C:59:ILE:O	1:C:426:LYS:NZ	2.47	0.46
1:C:20:TYR:CE2	1:C:28:ARG:HG3	2.51	0.46
2:B:494:LEU:C	2:B:494:LEU:HD23	2.36	0.46
1:C:431:PHE:HB2	9:C:667:HOH:O	2.14	0.46
1:C:253:TRP:CZ2	1:C:262:ILE:HG23	2.50	0.46
1:C:62:CYS:HB3	2:D:94:GLY:HA3	1.97	0.46
1:C:192:SER:CB	9:C:603:HOH:O	2.63	0.46
1:C:155:PRO:HB3	2:D:157:VAL:HG21	1.97	0.46
1:C:440:GLU:CG	9:C:766:HOH:O	2.61	0.45
2:B:88:TYR:O	2:B:149:VAL:HA	2.16	0.45
1:C:428:LYS:HG3	1:C:438:PHE:CD2	2.51	0.45
1:A:234:ASP:HB3	1:A:451:HIS:ND1	2.30	0.45
1:C:277:ARG:HD2	1:C:386:ASP:OD2	2.16	0.45
1:C:417:LYS:NZ	9:C:605:HOH:O	2.22	0.45
1:A:414:LYS:HG3	1:A:434:MET:HE1	1.99	0.45
1:A:399:LEU:HD12	1:A:400:LEU:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:ASP:O	2:D:26:LYS:HG2	2.17	0.45
2:B:270:ARG:NH2	9:B:720:HOH:O	2.50	0.45
2:D:151:THR:CG2	2:D:162:LEU:HD21	2.46	0.45
1:A:59:ILE:HD12	1:A:354:TYR:CE2	2.52	0.44
2:B:70:CYS:HB2	2:B:188:SER:HB2	1.98	0.44
1:C:296:GLU:HB3	9:C:727:HOH:O	2.16	0.44
1:A:440:GLU:HG2	9:A:785:HOH:O	2.08	0.44
1:C:265:THR:HB	1:C:266:PRO:HD3	1.99	0.44
2:B:445:ASN:HB2	2:B:472:PRO:O	2.17	0.44
1:C:276:TYR:OH	1:C:284:ARG:NH2	2.50	0.44
2:B:5:VAL:HG12	9:B:887:HOH:O	2.16	0.44
2:D:86:MET:HG2	2:D:138:CYS:SG	2.57	0.44
1:C:421:ILE:O	1:C:438:PHE:HA	2.17	0.44
1:A:93:ARG:HH21	5:B:608:GOL:HO2	1.63	0.44
1:C:82:SER:N	9:C:630:HOH:O	2.50	0.44
2:D:322:LEU:HD13	2:D:351:LEU:HD23	1.99	0.44
2:B:7:LYS:CD	9:B:946:HOH:O	2.66	0.44
2:B:132:LYS:HD3	2:B:174:PHE:CE2	2.53	0.44
1:C:382:ALA:HB3	1:C:387:TYR:CE2	2.53	0.44
5:B:605:GOL:H12	9:B:829:HOH:O	2.17	0.44
1:C:6:ARG:HG2	1:C:10:GLU:OE2	2.18	0.44
2:B:492:GLN:HB3	5:B:605:GOL:H31	2.00	0.44
1:A:381:PHE:HA	9:A:747:HOH:O	2.18	0.44
2:D:390:PRO:O	2:D:419:ALA:CB	2.65	0.43
2:B:194:VAL:HB	2:B:297:HIS:CG	2.53	0.43
5:B:606:GOL:H12	5:B:607:GOL:O2	2.18	0.43
1:C:234:ASP:HB3	1:C:451:HIS:CG	2.54	0.43
1:C:79:ILE:O	1:C:148:ILE:HA	2.18	0.43
2:B:86:MET:HG2	2:B:138:CYS:SG	2.58	0.43
1:C:9:VAL:HG12	1:C:34:VAL:HG22	2.01	0.43
1:C:62:CYS:HA	9:C:644:HOH:O	2.18	0.43
1:C:366:ALA:HB3	9:C:786:HOH:O	2.17	0.43
2:B:241:LYS:NZ	2:B:256:ASP:OD2	2.47	0.43
2:D:49:THR:HB	8:D:602:TRS:C3	2.49	0.43
1:C:9:VAL:O	1:C:13:ILE:HD13	2.19	0.43
2:B:90:HIS:CB	9:B:801:HOH:O	2.53	0.43
2:B:320:MET:SD	5:B:607:GOL:C3	3.07	0.43
2:D:317:ASN:ND2	9:D:725:HOH:O	2.52	0.43
1:C:405:THR:HG22	5:C:508:GOL:H32	2.01	0.43
1:C:196:HIS:ND1	9:C:606:HOH:O	2.22	0.43
1:A:112:MET:HA	5:B:608:GOL:HO2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:ALA:HB1	1:A:386:ASP:HB2	2.01	0.42
2:B:447:TYR:CD1	2:D:521:LEU:HD22	2.54	0.42
1:A:359:ARG:N	1:A:360:PRO:CD	2.82	0.42
1:C:184:GLU:HA	9:C:627:HOH:O	2.19	0.42
1:C:253:TRP:HA	1:C:254:SER:HA	1.75	0.42
2:D:494:LEU:HD23	2:D:494:LEU:C	2.40	0.42
2:D:352:VAL:O	2:D:356:THR:HG23	2.19	0.42
2:B:12:TYR:HA	2:B:13:PRO:HA	1.83	0.42
2:B:377:MET:HE2	2:B:377:MET:HB3	1.79	0.42
1:C:97:ARG:O	1:C:231:ILE:HA	2.19	0.42
2:D:156:GLU:HG3	2:D:187:PRO:HB3	2.01	0.42
2:B:123:ALA:HB2	2:B:154:MET:HE3	2.02	0.42
1:A:158:LEU:HD11	2:B:154:MET:HG3	2.01	0.42
1:C:364:ILE:HG12	1:C:374:VAL:HG21	2.01	0.42
2:D:240:ILE:HG13	2:D:293:LEU:HD11	2.01	0.42
2:B:470:GLY:N	9:B:725:HOH:O	2.52	0.42
1:C:399:LEU:HD12	1:C:400:LEU:H	1.85	0.42
2:D:154:MET:CG	9:D:773:HOH:O	2.68	0.42
1:A:399:LEU:HD12	1:A:400:LEU:N	2.35	0.42
2:B:50:LYS:HB2	8:B:604:TRS:HN1	1.84	0.42
1:C:86:VAL:O	1:C:86:VAL:HG22	2.19	0.42
2:B:470:GLY:CA	9:B:725:HOH:O	2.67	0.41
1:A:413:VAL:HG11	1:A:436:ILE:HD12	2.02	0.41
1:A:449:PRO:O	1:A:455:GLY:HA2	2.19	0.41
1:A:420:LEU:HB2	1:A:467:LEU:HD12	2.01	0.41
2:D:241:LYS:NZ	2:D:256:ASP:OD2	2.49	0.41
1:A:19:VAL:HG11	1:A:407:TYR:CZ	2.55	0.41
2:D:316:LEU:HD11	2:D:331:LYS:HG2	2.02	0.41
1:A:42:SER:OG	1:A:384:ASN:HB3	2.20	0.41
1:C:382:ALA:HB1	1:C:386:ASP:HB2	2.03	0.41
2:B:175:ILE:CD1	2:B:181:VAL:HG21	2.51	0.41
1:A:42:SER:CB	1:A:388:ASP:OD1	2.69	0.41
2:B:521:LEU:HD22	2:D:447:TYR:CD1	2.55	0.41
1:A:136:ASP:CG	1:A:170:LYS:HZ1	2.24	0.41
1:C:52:SER:HB3	5:C:508:GOL:C1	2.50	0.41
1:A:31:HIS:NE2	1:A:47:ILE:HD11	2.36	0.41
2:D:414:PRO:O	2:D:417:LYS:HG3	2.21	0.41
2:B:254:LEU:HD22	2:B:281:MET:SD	2.61	0.41
1:A:22:GLU:HG2	1:A:26:LYS:HE3	2.02	0.41
1:C:68:LYS:NZ	5:C:505:GOL:H31	2.35	0.41
1:A:467:LEU:HD23	1:A:467:LEU:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:SER:OG	1:C:448:GLY:N	2.53	0.41
1:C:422:GLY:HA2	1:C:439:ARG:O	2.21	0.41
1:C:62:CYS:SG	1:C:64:TYR:HB3	2.61	0.41
2:B:113:CYS:CB	9:B:947:HOH:O	2.69	0.41
2:B:296:TRP:CD1	2:B:377:MET:HE3	2.55	0.41
2:D:151:THR:HG22	2:D:162:LEU:HD21	2.03	0.41
1:C:440:GLU:HG3	9:C:609:HOH:O	2.20	0.41
1:C:39:VAL:HG23	1:C:391:MET:SD	2.61	0.41
1:C:22:GLU:OE2	1:C:25:ARG:NH2	2.54	0.41
1:C:68:LYS:HZ1	5:C:505:GOL:H31	1.86	0.41
2:B:151:THR:CG2	2:B:162:LEU:HD11	2.50	0.41
1:A:274:HIS:CD2	1:A:451:HIS:CE1	3.08	0.41
1:A:355:ILE:HB	1:A:360:PRO:HD3	2.02	0.41
2:B:48:THR:OG1	2:B:458:LYS:HE3	2.21	0.41
2:D:88:TYR:O	2:D:149:VAL:HA	2.21	0.41
1:A:428:LYS:CB	9:A:785:HOH:O	2.51	0.40
5:B:603:GOL:O2	2:D:514:ALA:O	2.35	0.40
1:C:135:ILE:HD13	1:C:178:ILE:HD13	2.03	0.40
1:A:253:TRP:CZ2	1:A:262:ILE:HG23	2.57	0.40
2:B:375:PHE:HD1	5:B:607:GOL:C3	2.35	0.40
2:D:449:LYS:HB2	2:D:449:LYS:HE3	1.79	0.40
1:C:379:TYR:CG	1:C:382:ALA:HB2	2.57	0.40
1:A:277:ARG:HD2	1:A:386:ASP:OD2	2.20	0.40
1:A:97:ARG:O	1:A:231:ILE:HA	2.22	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	479/490 (98%)	457 (95%)	20 (4%)	2 (0%)	39 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	477/490 (97%)	448 (94%)	29 (6%)	0	100	100
2	B	521/522 (100%)	504 (97%)	16 (3%)	1 (0%)	52	47
2	D	520/522 (100%)	501 (96%)	18 (4%)	1 (0%)	52	47
All	All	1997/2024 (99%)	1910 (96%)	83 (4%)	4 (0%)	52	47

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	ALA
2	B	255	SER
2	D	255	SER
1	A	355	ILE

5.3.2 Protein sidechains

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	409/413 (99%)	405 (99%)	4 (1%)	82	84
1	C	408/413 (99%)	402 (98%)	6 (2%)	72	73
2	B	455/454 (100%)	452 (99%)	3 (1%)	88	90
2	D	454/454 (100%)	450 (99%)	4 (1%)	84	86
All	All	1726/1734 (100%)	1709 (99%)	17 (1%)	82	84

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	SER
1	A	98	ASN
1	A	362	HIS
1	A	401	TYR
2	B	177	ASP
2	B	258	GLU
2	B	449	LYS

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Mol	Chain	Res	Type
1	C	43	LYS
1	C	98	ASN
1	C	279	MET
1	C	362	HIS
1	C	401	TYR
1	C	445	ASP
2	D	88	TYR
2	D	102	TYR
2	D	172	GLU
2	D	258	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	HIS
1	A	384	ASN
2	B	65	ASN
1	C	98	ASN
1	C	321	GLN
1	C	384	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 for Mogul analysis.

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	$\#\|Z\| > 2$
3	HCA	A	501	-	4,13,13	0.83	0	3,18,18	1.42	1 (33%)
4	ICS	A	502	1	6,30,30	1.69	1 (16%)	0,78,78	0.00	-
5	GOL	A	503	-	5,5,5	0.20	0	5,5,5	0.56	0
6	1CL	A	504	1,2	0,22,22	0.00	-	0,44,44	0.00	-
5	GOL	B	602	-	5,5,5	0.63	0	5,5,5	0.78	0
5	GOL	B	603	-	5,5,5	0.51	0	5,5,5	0.72	0
8	TRS	B	604	-	7,7,7	0.88	0	9,9,9	1.71	2 (22%)
5	GOL	B	605	-	5,5,5	0.23	0	5,5,5	0.76	0
5	GOL	B	606	-	5,5,5	0.38	0	5,5,5	0.88	0
5	GOL	B	607	-	5,5,5	0.28	0	5,5,5	0.93	0
5	GOL	B	608	-	5,5,5	1.09	1 (20%)	5,5,5	2.14	1 (20%)
3	HCA	C	501	-	4,13,13	0.84	0	3,18,18	2.04	1 (33%)
4	ICS	C	502	1	6,30,30	2.37	3 (50%)	0,78,78	0.00	-
5	GOL	C	503	-	5,5,5	0.44	0	5,5,5	1.32	1 (20%)
5	GOL	C	504	-	5,5,5	0.40	0	5,5,5	0.54	0
5	GOL	C	505	-	5,5,5	0.98	1 (20%)	5,5,5	1.59	1 (20%)
5	GOL	C	506	-	5,5,5	0.45	0	5,5,5	0.52	0
5	GOL	C	507	-	5,5,5	0.86	0	5,5,5	1.24	0
5	GOL	C	508	-	5,5,5	0.61	0	5,5,5	0.71	0
6	1CL	C	509	1,2	0,22,22	0.00	-	0,44,44	0.00	-
5	GOL	D	601	-	5,5,5	0.37	0	5,5,5	0.24	0
8	TRS	D	602	-	7,7,7	0.64	0	9,9,9	1.05	0
5	GOL	D	603	-	5,5,5	0.36	0	5,5,5	0.36	0

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
3	HCA	A	501	-	-	0/7/17/17	0/0/0/0
4	ICS	A	502	1	-	0/0/204/204	0/0/13/13
5	GOL	A	503	-	-	0/4/4/4	0/0/0/0
6	1CL	A	504	1,2	-	0/0/88/88	0/6/8/8
5	GOL	B	602	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	603	-	-	0/4/4/4	0/0/0/0
8	TRS	B	604	-	-	0/9/9/9	0/0/0/0
5	GOL	B	605	-	-	0/4/4/4	0/0/0/0
5	GOL	B	606	-	-	0/4/4/4	0/0/0/0
5	GOL	B	607	-	-	0/4/4/4	0/0/0/0
5	GOL	B	608	-	-	0/4/4/4	0/0/0/0
3	HCA	C	501	-	-	0/7/17/17	0/0/0/0
4	ICS	C	502	1	-	0/0/204/204	0/0/13/13
5	GOL	C	503	-	-	0/4/4/4	0/0/0/0
5	GOL	C	504	-	-	0/4/4/4	0/0/0/0
5	GOL	C	505	-	-	0/4/4/4	0/0/0/0
5	GOL	C	506	-	-	0/4/4/4	0/0/0/0
5	GOL	C	507	-	-	0/4/4/4	0/0/0/0
5	GOL	C	508	-	-	0/4/4/4	0/0/0/0
6	1CL	C	509	1,2	-	0/0/88/88	0/6/8/8
5	GOL	D	601	-	-	0/4/4/4	0/0/0/0
8	TRS	D	602	-	-	0/9/9/9	0/0/0/0
5	GOL	D	603	-	-	0/4/4/4	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	502	ICS	S5A-FE3	-3.95	2.15	2.24
4	C	502	ICS	S3A-FE4	-3.56	2.16	2.24
4	A	502	ICS	S5A-FE3	-3.38	2.16	2.24
4	C	502	ICS	S3A-FE5	-2.10	2.19	2.24
5	C	505	GOL	O2-C2	2.01	1.49	1.43
5	B	608	GOL	O3-C3	2.42	1.52	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	501	HCA	C3-C2-C1	-2.89	110.43	114.95
3	A	501	HCA	C3-C2-C1	-2.42	111.17	114.95
5	C	503	GOL	O2-C2-C3	2.07	118.42	108.47
5	C	505	GOL	O3-C3-C2	2.18	121.04	109.97
8	B	604	TRS	O3-C3-C	2.46	116.77	110.92
8	B	604	TRS	C3-C-N	3.52	113.86	107.88
5	B	608	GOL	C3-C2-C1	3.55	126.00	111.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	HCA	1	0
5	B	602	GOL	1	0
5	B	603	GOL	3	0
8	B	604	TRS	2	0
5	B	605	GOL	2	0
5	B	606	GOL	1	0
5	B	607	GOL	4	0
5	B	608	GOL	7	0
3	C	501	HCA	2	0
5	C	504	GOL	3	0
5	C	505	GOL	4	0
5	C	507	GOL	2	0
5	C	508	GOL	10	0
8	D	602	TRS	1	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	479/490 (97%)	0.87	56 (11%) 6 7	24, 39, 65, 100	12 (2%)
1	C	478/490 (97%)	1.11	77 (16%) 3 3	28, 46, 76, 93	4 (0%)
2	B	522/522 (100%)	0.45	22 (4%) 40 44	24, 36, 53, 70	5 (0%)
2	D	522/522 (100%)	0.44	21 (4%) 42 46	22, 37, 55, 80	13 (2%)
All	All	2001/2024 (98%)	0.70	176 (8%) 12 15	22, 39, 64, 100	34 (1%)

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	123	ALA	8.0
2	B	123	ALA	5.8
2	D	121	ASP	5.5
1	C	39	VAL	5.4
1	A	3	GLY	5.1
1	C	14	GLN	5.0
1	A	481	ALA	4.5
1	C	172	ALA	4.4
1	C	318	GLU	4.3
1	A	39	VAL	4.2
1	C	217	ALA	4.1
1	C	168	LYS	4.0
1	C	36	ASP	4.0
2	B	121	ASP	3.9
1	A	92	SER	3.9
1	C	7	GLU	3.7
1	A	124	VAL	3.7
2	B	178	GLU	3.6
2	B	101	SER	3.6
1	A	18	GLU	3.6
1	C	125	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	92	SER	3.6
1	C	392	LYS	3.6
1	C	443[A]	SER	3.5
1	C	322	LYS	3.5
1	C	317	ASP	3.4
1	C	59	ILE	3.4
2	B	177	ASP	3.4
1	C	44	LYS	3.4
1	C	75	ILE	3.4
1	C	292	ILE	3.4
2	D	215	ASP	3.4
1	C	221	TYR	3.3
1	A	125	PHE	3.3
1	A	75	ILE	3.3
1	A	212	GLU	3.3
1	A	40	THR	3.2
2	B	215	ASP	3.2
2	B	312	GLU	3.2
1	A	59	ILE	3.2
2	B	214	ASP	3.2
1	C	70	VAL	3.2
1	C	163	ILE	3.2
2	B	521	LEU	3.2
1	C	18	GLU	3.1
2	D	125	PHE	3.1
1	A	43	LYS	3.1
1	A	322	LYS	3.1
1	A	231	ILE	3.1
1	C	257	GLY	3.1
1	C	24	ALA	3.1
1	C	231	ILE	3.1
1	A	19	VAL	3.1
1	C	15	GLU	3.1
1	A	391	MET	3.1
1	A	70	VAL	3.0
1	A	392	LYS	3.0
2	D	417	LYS	3.0
2	B	96	VAL	3.0
1	A	45	CYS	3.0
1	A	409	PHE	3.0
2	D	101	SER	3.0
1	C	291	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	96	VAL	3.0
1	C	194	GLY	2.9
2	B	417	LYS	2.9
2	B	124	VAL	2.9
1	A	44	LYS	2.9
1	C	162	ASP	2.9
1	A	443[A]	SER	2.9
1	C	391	MET	2.9
1	A	168	LYS	2.9
1	C	43	LYS	2.9
1	C	40	THR	2.8
1	A	38	ALA	2.8
1	A	215	THR	2.8
2	D	521	LEU	2.8
2	B	173	GLY	2.7
1	C	425	ILE	2.7
2	D	217	VAL	2.7
1	A	7	GLU	2.7
1	A	279	MET	2.7
1	C	320	ILE	2.7
2	D	124	VAL	2.7
1	A	174	LEU	2.7
1	C	319	SER	2.7
2	B	125	PHE	2.7
1	C	94	ALA	2.6
1	A	318	GLU	2.6
2	D	38	ASP	2.6
1	C	176	LYS	2.6
2	D	102	TYR	2.6
1	C	321	GLN	2.6
2	B	38	ASP	2.6
1	C	212	GLU	2.6
1	C	476	GLN	2.6
1	A	172	ALA	2.6
1	A	72	TRP	2.6
1	A	41	GLN	2.6
1	A	42	SER	2.5
1	C	161	ASP	2.5
1	A	291	GLY	2.5
1	C	200	ASP	2.5
1	C	409	PHE	2.5
2	B	447	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	450	PHE	2.5
1	C	46	ILE	2.4
1	C	259	ILE	2.4
1	C	110	VAL	2.4
1	C	157	GLY	2.4
2	B	168	ASN	2.4
1	C	400	LEU	2.4
1	C	288	GLU	2.4
2	D	157	VAL	2.4
1	C	366	ALA	2.4
1	C	3	GLY	2.4
1	C	69	GLY	2.4
1	C	98	ASN	2.4
2	D	89	VAL	2.4
1	C	316	PHE	2.4
1	A	8	GLU	2.3
1	A	126	GLY	2.3
1	C	41	GLN	2.3
2	D	214	ASP	2.3
1	A	93	ARG	2.3
1	C	475	LEU	2.3
1	C	175	SER	2.3
1	C	37	PRO	2.2
1	C	123	ILE	2.2
2	D	46	TRP	2.2
1	A	36	ASP	2.2
1	C	16	VAL	2.2
1	A	257	GLY	2.2
2	B	450	PHE	2.2
2	B	261	LEU	2.2
1	A	477	ALA	2.2
1	A	15	GLU	2.2
2	D	265	ALA	2.2
1	A	110	VAL	2.2
1	C	71	VAL	2.2
1	A	449	PRO	2.1
1	C	190	SER	2.1
1	C	174	LEU	2.1
2	D	122	ALA	2.1
1	A	407	TYR	2.1
1	C	356	GLY	2.1
1	C	93	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	327	VAL	2.1
1	C	225	ILE	2.1
1	C	397	SER	2.1
1	A	213	ASP	2.1
2	B	102	TYR	2.1
1	C	4	MET	2.1
1	C	477	ALA	2.1
2	D	261	LEU	2.1
1	A	4	MET	2.1
1	A	112	MET	2.1
1	C	72	TRP	2.1
1	A	5	SER	2.1
1	A	11	SER	2.1
1	A	175	SER	2.1
1	C	45	CYS	2.1
1	C	56	LEU	2.1
1	A	397	SER	2.0
1	A	9	VAL	2.0
1	A	94	ALA	2.0
1	C	253	TRP	2.0
1	C	314	ALA	2.0
2	B	77	LEU	2.0
1	C	128	ASP	2.0
2	B	153	CYS	2.0
2	D	168	ASN	2.0
1	A	217	ALA	2.0
1	A	314	ALA	2.0
1	C	480	GLU	2.0
1	A	173	GLU	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
5	GOL	C	508	6/6	0.62	0.44	9.66	54,63,70,81	0
5	GOL	B	607	6/6	0.92	0.32	7.74	35,45,51,52	0
5	GOL	B	608	6/6	0.83	0.33	3.58	24,35,53,63	0
5	GOL	B	606	6/6	0.86	0.22	3.37	47,53,57,69	0
5	GOL	C	506	6/6	0.85	0.33	3.32	57,72,80,83	0
5	GOL	C	505	6/6	0.71	0.35	2.88	34,43,48,52	0
5	GOL	D	603	6/6	0.85	0.16	1.94	39,48,53,54	0
5	GOL	C	507	6/6	0.73	0.20	1.38	49,52,57,59	0
5	GOL	B	605	6/6	0.90	0.12	0.54	37,46,53,53	0
5	GOL	B	603	6/6	0.80	0.15	0.23	37,38,40,46	0
5	GOL	A	503	6/6	0.72	0.18	-0.39	39,42,44,44	0
3	HCA	A	501	14/14	0.91	0.15	-0.83	27,30,39,39	0
3	HCA	C	501	14/14	0.92	0.15	-1.35	28,34,39,39	0
6	1CL	C	509	15/15	0.93	0.08	-2.14	28,31,40,42	0
6	1CL	A	504	15/15	0.93	0.08	-2.29	26,30,37,41	15
4	ICS	A	502	18/18	0.98	0.06	-2.69	25,32,35,37	0
4	ICS	C	502	18/18	0.98	0.07	-3.03	28,33,39,40	0
7	CA	B	601	1/1	0.99	0.04	-5.03	41,41,41,41	0
7	CA	B	609	1/1	0.94	0.04	-5.81	42,42,42,42	0
5	GOL	D	601	6/6	0.75	0.17	-	54,57,59,65	0
5	GOL	C	504	6/6	0.76	0.20	-	42,51,56,58	0
8	TRS	B	604	8/8	0.65	0.25	-	53,60,71,72	0
8	TRS	D	602	8/8	0.74	0.20	-	52,60,65,66	0
5	GOL	B	602	6/6	0.71	0.26	-	40,48,53,55	0
5	GOL	C	503	6/6	0.71	0.21	-	48,58,61,63	0

6.5 Other polymers (i)

There are no such residues in this entry.