Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:56 AM GMT

PDB ID	:	2OOV
Title	:	Crystal Structure of Hansenula polymorpha amine oxidase to 1.7 Angstroms
Authors	:	Johnson, B.J.; Wilmot, C.M.
Deposited on	:	2007-01-26
Resolution	:	1.70 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:

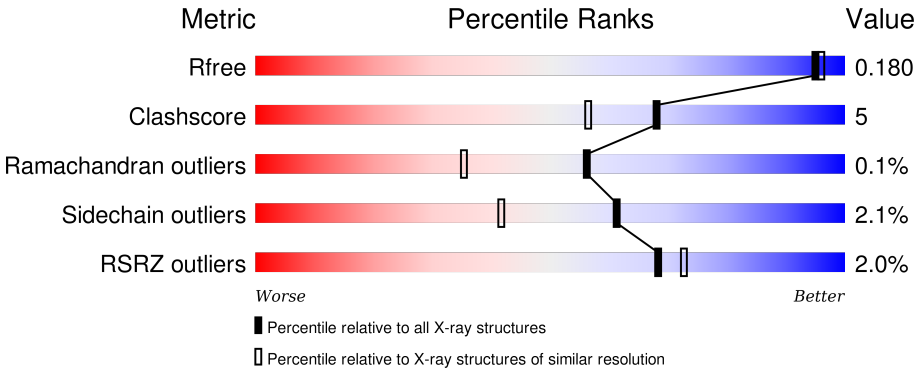
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	660	2% 91% 7% ••
1	B	660	2% 91% 7% ••
2	C	660	2% 91% 7% ••
2	D	660	2% 89% 9% ••
2	E	660	2% 92% 7% •

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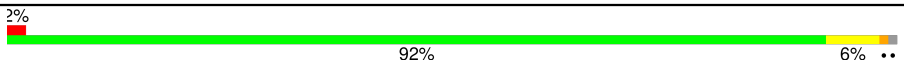
Mol	Chain	Length	Quality of chain
2	F	660	

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	A	6012	-	-	-	X
5	GOL	A	6013	-	-	-	X
5	GOL	A	6017	-	-	-	X
5	GOL	A	6027	-	-	-	X
5	GOL	B	6009	-	-	-	X
5	GOL	B	6023	-	-	-	X
5	GOL	B	6024	-	-	-	X
5	GOL	B	6025	-	-	-	X
5	GOL	C	6002	-	-	-	X
5	GOL	C	6007	-	-	-	X
5	GOL	C	6021	-	-	-	X
5	GOL	C	6029	-	-	-	X
5	GOL	D	6028	-	-	X	X
5	GOL	E	6014	-	-	-	X
5	GOL	E	6015	-	-	-	X
5	GOL	E	6016	-	-	-	X
5	GOL	E	6019	-	-	-	X
5	GOL	E	6020	-	-	-	X
5	GOL	E	6022	-	-	-	X
5	GOL	F	6001	-	-	-	X
5	GOL	F	6003	-	-	-	X
5	GOL	F	6006	-	-	-	X
5	GOL	F	6008	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36770 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 Peroxisomal copper amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	655	Total	C	N	O	S	0	13	0
			5253	3347	896	986	24			
1	B	655	Total	C	N	O	S	0	10	0
			5235	3333	894	982	26			

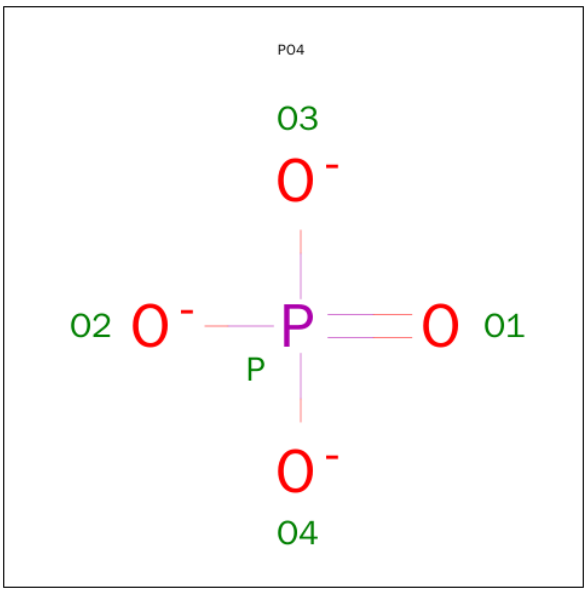
- Molecule 2 is a protein called Peroxisomal copper amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	655	Total	C	N	O	S	0	17	0
			5288	3369	899	991	29			
2	D	655	Total	C	N	O	S	0	14	0
			5266	3361	894	984	27			
2	E	655	Total	C	N	O	S	0	9	0
			5244	3338	895	986	25			
2	F	655	Total	C	N	O	S	0	10	0
			5245	3340	895	982	28			

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

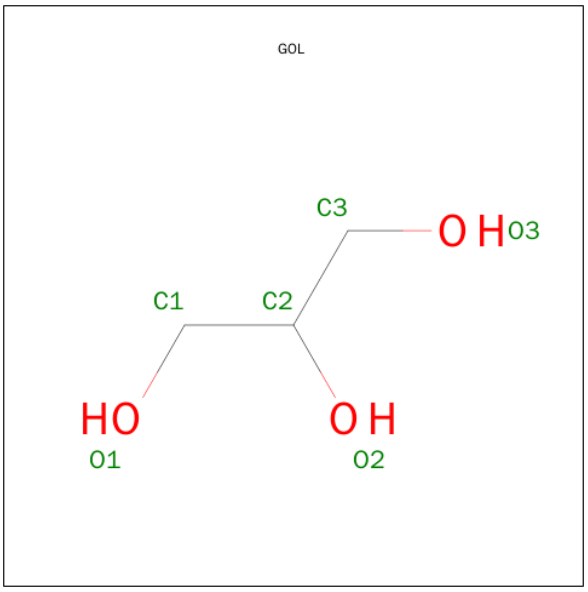
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Cu	0	0
			1	1		
3	E	1	Total	Cu	0	0
			1	1		
3	B	1	Total	Cu	0	0
			1	1		
3	C	1	Total	Cu	0	0
			1	1		
3	A	1	Total	Cu	0	0
			1	1		
3	F	1	Total	Cu	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O P 5 4 1	0	0
4	F	1	Total O P 5 4 1	0	0

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



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

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

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

- Molecule 6 is water.

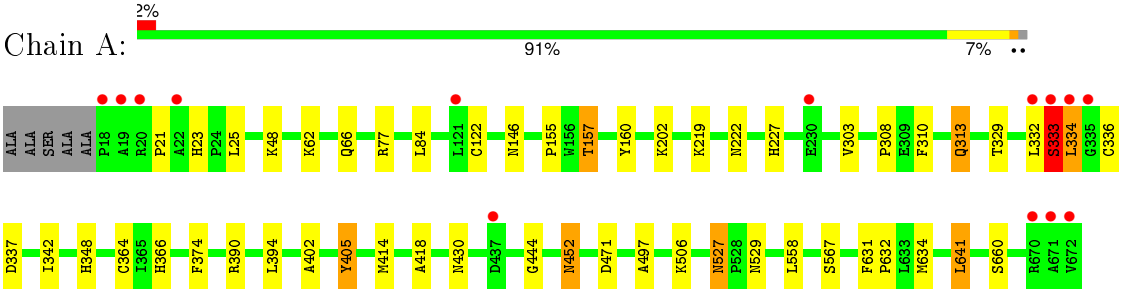
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	852	Total	O	0	0
			852	852		
6	B	816	Total	O	0	0
			816	816		
6	C	849	Total	O	0	0
			849	849		
6	D	863	Total	O	0	0
			863	863		
6	E	853	Total	O	0	0
			853	853		
6	F	822	Total	O	0	0
			822	822		

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.

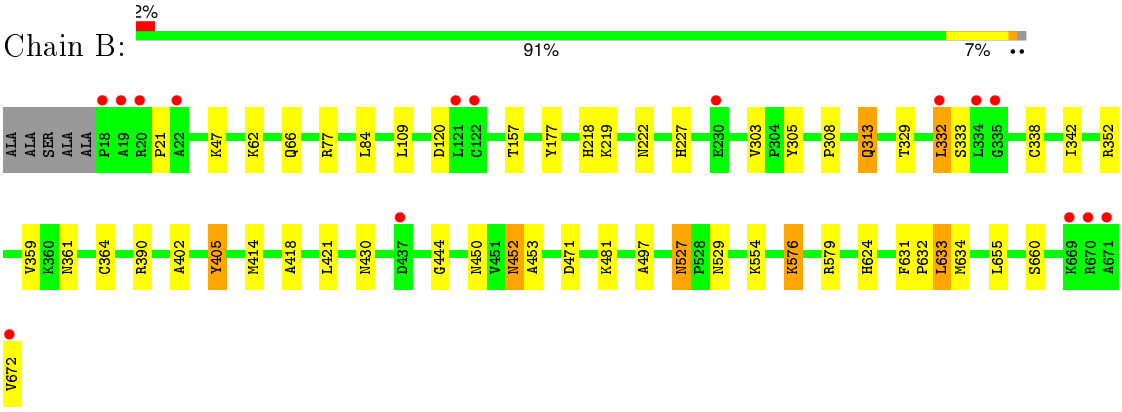
- Molecule 1: Peroxisomal copper amine oxidase

Chain A:



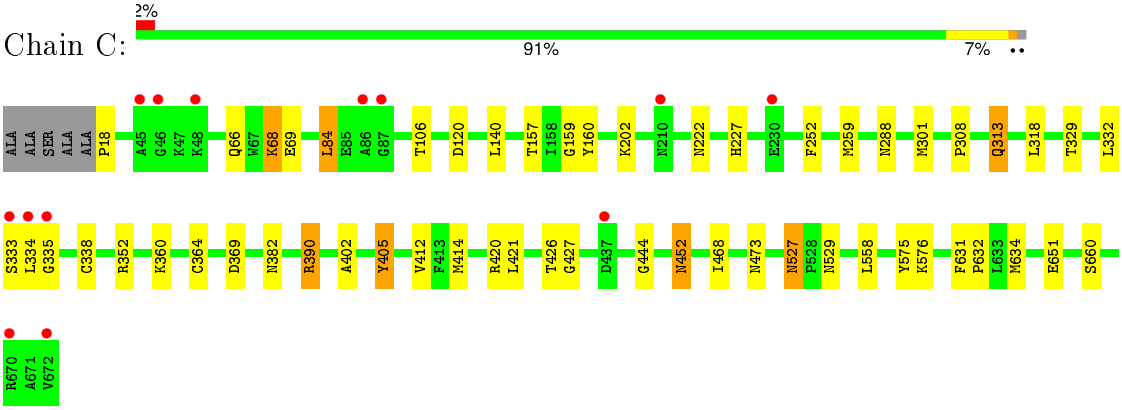
- Molecule 1: Peroxisomal copper amine oxidase

Chain B:



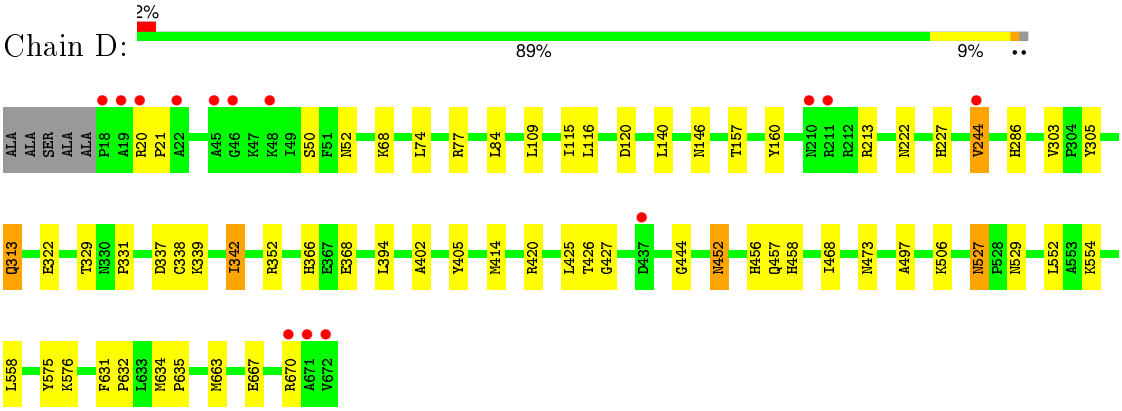
- Molecule 2: Peroxisomal copper amine oxidase

Chain C:



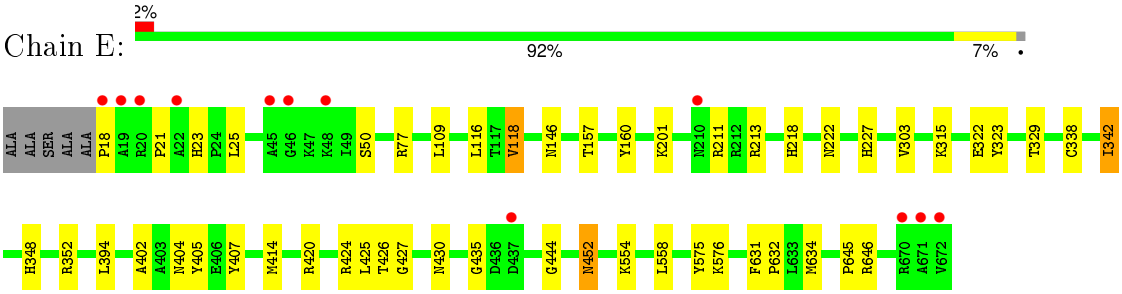
• Molecule 2: Peroxisomal copper amine oxidase

Chain D:



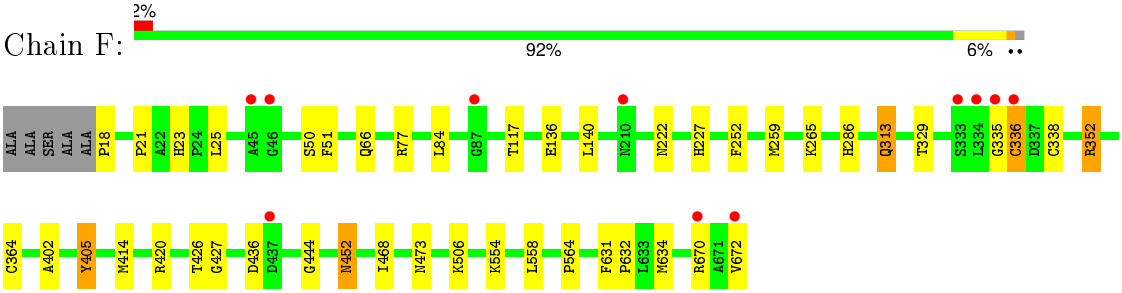
• Molecule 2: Peroxisomal copper amine oxidase

Chain E:



• Molecule 2: Peroxisomal copper amine oxidase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	104.15Å 223.08Å 104.25Å 90.00° 95.77° 90.00°	Depositor
Resolution (Å)	37.96 – 1.70 37.96 – 1.70	Depositor EDS
% Data completeness (in resolution range)	85.0 (37.96-1.70) 85.0 (37.96-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.147 , 0.178 0.150 , 0.180	Depositor DCC
R_{free} test set	21965 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	15.4	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.4	EDS
Estimated twinning fraction	0.477 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 437276 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	36770	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: GOL, PO4, CU, SME, TPQ

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	0.53	0/5417	0.64	2/7364 (0.0%)
1	B	0.53	0/5390	0.63	0/7330
2	C	0.52	0/5451	0.63	1/7413 (0.0%)
2	D	0.53	0/5426	0.64	0/7382
2	E	0.53	0/5386	0.64	0/7328
2	F	0.53	0/5393	0.62	0/7336
All	All	0.53	0/32463	0.63	3/44153 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
2	C	0	1
2	F	0	1
All	All	0	6

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	334	LEU	N-CA-C	-7.43	90.94	111.00
1	A	641	LEU	CA-CB-CG	6.30	129.80	115.30
2	C	84	LEU	CA-CB-CG	5.83	128.71	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	332	LEU	Peptide
1	A	333	SER	Peptide
1	A	405	TPQ	Mainchain
1	B	405	TPQ	Mainchain
2	C	405[A]	TPQ	Mainchain
2	F	405[A]	TPQ	Mainchain

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	5253	0	5125	46	0
1	B	5235	0	5095	42	0
2	C	5288	0	5148	49	0
2	D	5266	0	5137	59	0
2	E	5244	0	5087	49	0
2	F	5245	0	5095	43	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	C	5	0	0	0	0
4	F	5	0	0	0	0
5	A	36	0	48	6	0
5	B	36	0	48	2	0
5	C	24	0	32	2	0
5	D	12	0	16	9	0
5	E	36	0	48	2	0
5	F	24	0	32	4	0
6	A	852	0	0	16	0
6	B	816	0	0	5	0
6	C	849	0	0	10	0
6	D	863	0	0	16	0
6	E	853	0	0	15	0
6	F	822	0	0	8	0
All	All	36770	0	30911	287	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 5.

All (287) 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)
2:E:404:ASN:C	2:E:405[A]:TPQ:H2	1.08	1.53
2:E:404:ASN:C	2:E:405[B]:TPQ:H2	0.96	1.49
2:D:157[A]:THR:CG2	6:D:6597:HOH:O	1.75	1.34
1:A:157[B]:THR:CG2	6:A:6465:HOH:O	1.72	1.34
2:E:157[B]:THR:CG2	6:E:6588:HOH:O	1.74	1.25
2:D:157[B]:THR:OG1	6:D:6597:HOH:O	1.53	1.21
2:D:157[A]:THR:OG1	6:D:6603:HOH:O	1.56	1.21
2:E:157[A]:THR:OG1	6:E:6588:HOH:O	1.58	1.18
2:E:157[B]:THR:OG1	6:E:6598:HOH:O	1.64	1.11
2:C:333:SER:HB2	2:C:334:LEU:HG	1.36	1.08
2:D:405[B]:TPQ:O5	2:D:634[B]:MET:HE3	1.57	1.02
2:F:352:ARG:HH11	2:F:352:ARG:HG3	1.20	1.02
2:E:405[A]:TPQ:O5	2:E:634[A]:MET:SD	2.17	1.01
2:C:334:LEU:N	2:C:335:GLY:HA2	1.77	0.99
2:D:405[B]:TPQ:O5	2:D:634[B]:MET:CE	2.09	0.99
2:C:288:ASN:HB2	6:C:6460:HOH:O	1.63	0.97
2:D:425[B]:LEU:HD21	6:D:6751:HOH:O	1.62	0.96
2:C:157[B]:THR:OG1	6:C:6628:HOH:O	1.82	0.96
2:D:338:CYS:SG	2:D:342:ILE:HG12	2.06	0.95
2:E:338:CYS:SG	2:E:342:ILE:HG12	2.06	0.94
1:A:157[B]:THR:HG22	6:A:6465:HOH:O	1.52	0.87
1:A:23:HIS:HD2	1:A:25:LEU:H	1.21	0.87
1:A:333:SER:HB3	1:A:337:ASP:OD1	1.77	0.84
2:E:23:HIS:HD2	2:E:25:LEU:H	1.21	0.84
2:E:157[B]:THR:HG23	6:E:6588:HOH:O	1.55	0.84
2:D:157[A]:THR:HG22	6:D:6597:HOH:O	1.50	0.83
2:D:425[B]:LEU:CD2	6:D:6751:HOH:O	2.22	0.82
2:E:157[A]:THR:HG21	2:E:322:GLU:HB3	1.62	0.81
1:B:157:THR:HG22	6:B:6594:HOH:O	1.79	0.81
2:F:352:ARG:HG3	2:F:352:ARG:NH1	1.93	0.81
2:F:23:HIS:HD2	2:F:25:LEU:H	1.28	0.80
2:E:157[B]:THR:HG22	6:E:6588:HOH:O	1.56	0.80
1:B:157:THR:CG2	6:B:6594:HOH:O	2.31	0.79
2:F:468:ILE:H	2:F:473:ASN:HD21	1.29	0.79
5:D:6028:GOL:H11	6:D:6662:HOH:O	1.84	0.77
2:C:468:ILE:H	2:C:473:ASN:HD21	1.32	0.76
2:D:405[B]:TPQ:O5	2:D:634[B]:MET:HE1	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:20:ARG:HG2	5:D:6028:GOL:H32	1.69	0.74
1:A:567[B]:SER:OG	6:A:6672:HOH:O	2.07	0.72
2:D:157[B]:THR:HG21	2:D:322:GLU:HB3	1.71	0.71
2:E:315:LYS:NZ	2:E:430:ASN:HD21	1.89	0.71
2:E:348:HIS:HD2	6:E:6258:HOH:O	1.73	0.70
2:F:414[A]:MET:SD	2:F:420:ARG:NH1	2.65	0.70
2:D:21:PRO:HD2	5:D:6028:GOL:H2	1.73	0.70
2:E:116:LEU:HD12	2:E:157[A]:THR:HG22	1.73	0.69
2:C:160:TYR:CD2	2:C:558:LEU:HD21	2.27	0.69
2:D:468:ILE:H	2:D:473:ASN:HD21	1.41	0.68
1:A:527:ASN:HD22	1:A:529:ASN:H	1.40	0.67
2:C:333:SER:HB2	2:C:334:LEU:CG	2.21	0.67
2:C:68:LYS:HD2	2:C:69:GLU:HG3	1.76	0.66
1:B:527:ASN:HD22	1:B:529:ASN:H	1.43	0.66
2:E:315:LYS:HZ2	2:E:430:ASN:HD21	1.43	0.66
2:D:402:ALA:O	2:D:405[A]:TPQ:H6	1.96	0.65
2:D:74:LEU:HD21	5:D:6028:GOL:H12	1.79	0.65
2:E:23:HIS:CD2	2:E:25:LEU:H	2.10	0.65
2:F:338:CYS:HG	2:F:364[B]:CYS:CB	2.10	0.64
2:D:157[A]:THR:HG23	6:D:6597:HOH:O	1.64	0.64
1:A:471:ASP:OD1	6:A:6575:HOH:O	2.14	0.64
2:D:527:ASN:HD22	2:D:529:ASN:H	1.46	0.62
2:D:116:LEU:HD12	2:D:157[B]:THR:HG22	1.80	0.62
2:C:651:GLU:HG2	5:C:6021:GOL:H31	1.81	0.62
1:B:402:ALA:O	1:B:405:TPQ:H6	1.99	0.62
2:C:390[A]:ARG:HG3	2:C:660:SER:OG	1.99	0.62
1:A:506[B]:LYS:NZ	6:A:6790:HOH:O	2.33	0.62
2:C:338:CYS:HG	2:C:364[B]:CYS:CB	2.13	0.62
2:E:50:SER:HB2	2:E:352:ARG:HG3	1.82	0.61
2:C:575:TYR:O	2:C:576:LYS:HD2	2.00	0.61
1:A:402:ALA:O	1:A:405:TPQ:H6	2.00	0.61
2:F:338:CYS:HB3	2:F:364[B]:CYS:HG	1.65	0.61
2:C:527:ASN:HD22	2:C:529:ASN:H	1.48	0.60
2:E:402:ALA:O	2:E:405[B]:TPQ:H6	2.01	0.60
2:E:315:LYS:HZ2	2:E:430:ASN:ND2	1.99	0.60
2:C:338:CYS:HB3	2:C:364[B]:CYS:SG	2.42	0.60
2:E:218:HIS:HD2	5:E:6015:GOL:H31	1.67	0.60
2:C:338:CYS:HB3	2:C:364[B]:CYS:HG	1.67	0.59
2:C:334:LEU:N	2:C:335:GLY:CA	2.56	0.59
1:A:23:HIS:CD2	1:A:25:LEU:H	2.13	0.59
2:F:402:ALA:O	2:F:405[A]:TPQ:H6	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:333:SER:C	2:C:335:GLY:HA2	2.23	0.58
1:B:177:TYR:OH	5:B:6023:GOL:H11	2.03	0.58
1:B:338:CYS:HG	1:B:364[B]:CYS:CB	2.15	0.58
6:A:6490:HOH:O	1:B:554:LYS:HE3	2.03	0.58
2:F:338:CYS:HB3	2:F:364[B]:CYS:SG	2.43	0.58
2:C:527:ASN:HD22	2:C:527:ASN:C	2.06	0.58
2:E:414[A]:MET:SD	2:E:420:ARG:NH1	2.77	0.58
1:B:21:PRO:HG3	1:B:77:ARG:CZ	2.34	0.58
1:A:348:HIS:HD2	6:A:6111:HOH:O	1.86	0.58
2:C:332:LEU:O	2:C:333:SER:HB3	2.03	0.58
2:F:50:SER:HB2	2:F:352:ARG:HG2	1.84	0.58
1:A:313:GLN:H	1:A:313:GLN:HE21	1.50	0.58
2:D:338:CYS:SG	2:D:342:ILE:CG1	2.90	0.56
2:E:218:HIS:HE1	6:E:6307:HOH:O	1.87	0.56
1:A:157[B]:THR:HG21	6:A:6465:HOH:O	1.65	0.56
2:F:468:ILE:H	2:F:473:ASN:ND2	2.01	0.56
2:E:634[B]:MET:HE1	6:E:6752:HOH:O	2.05	0.56
1:B:576:LYS:HE3	1:B:579:ARG:NH2	2.20	0.56
2:E:157[A]:THR:HB	6:E:6598:HOH:O	2.04	0.55
2:C:160:TYR:HD2	2:C:558:LEU:HD21	1.71	0.55
2:F:427:GLY:O	2:F:634[A]:MET:HG2	2.06	0.55
2:F:335:GLY:C	2:F:336[B]:CYS:SG	2.85	0.55
2:C:402:ALA:O	2:C:405[A]:TPQ:H6	2.07	0.55
2:D:50:SER:HB2	2:D:352:ARG:HG3	1.87	0.55
1:B:313:GLN:HE21	1:B:313:GLN:H	1.53	0.54
1:A:155:PRO:C	6:A:6771:HOH:O	2.46	0.54
2:D:157[B]:THR:HB	6:D:6603:HOH:O	2.06	0.54
5:D:6028:GOL:O2	6:D:6304:HOH:O	2.18	0.54
1:B:342:ILE:HG23	1:B:364[B]:CYS:SG	2.48	0.54
2:D:527:ASN:C	2:D:527:ASN:HD22	2.11	0.53
2:C:18:PRO:N	6:C:6453:HOH:O	2.40	0.53
2:C:338:CYS:CB	2:C:364[B]:CYS:SG	2.97	0.53
2:F:338:CYS:SG	2:F:364[B]:CYS:SG	3.07	0.53
1:B:624:HIS:CE1	1:B:634:SME:HE3	2.44	0.53
2:D:366:HIS:NE2	2:D:368:GLU:OE1	2.37	0.53
2:F:313:GLN:HE21	2:F:313:GLN:H	1.55	0.52
2:F:444:GLY:HA3	2:F:452:ASN:HD21	1.74	0.52
1:B:527:ASN:C	1:B:527:ASN:HD22	2.12	0.52
2:D:414[A]:MET:SD	2:D:420:ARG:NH1	2.83	0.52
2:D:50:SER:HB2	2:D:352:ARG:CG	2.40	0.52
2:F:564:PRO:HG3	6:F:6661:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:338:CYS:CB	2:C:364[B]:CYS:HG	2.23	0.51
2:C:427:GLY:O	2:C:634[A]:MET:HG2	2.10	0.51
2:F:136:GLU:HG3	6:F:6267:HOH:O	2.10	0.51
1:A:21:PRO:HG3	1:A:77:ARG:CZ	2.39	0.51
2:D:74:LEU:CD2	5:D:6028:GOL:H31	2.40	0.51
1:A:527:ASN:ND2	1:A:529:ASN:H	2.08	0.51
2:D:313:GLN:H	2:D:313:GLN:HE21	1.59	0.51
2:D:575:TYR:O	2:D:576:LYS:HD2	2.10	0.51
1:A:23:HIS:HE1	6:A:6342:HOH:O	1.93	0.51
1:B:338:CYS:HG	1:B:364[B]:CYS:HB3	1.75	0.51
2:D:527:ASN:HD21	2:D:529:ASN:HB2	1.75	0.51
2:F:313:GLN:NE2	2:F:313:GLN:H	2.08	0.51
2:E:222:ASN:HB3	2:E:227:HIS:CG	2.45	0.51
2:D:21:PRO:HG3	2:D:77:ARG:CZ	2.41	0.51
2:D:120:ASP:OD2	2:D:352:ARG:NH2	2.43	0.51
2:E:211:ARG:NH2	2:E:435:GLY:HA3	2.26	0.51
2:D:160:TYR:CD2	2:D:558:LEU:HD21	2.46	0.51
1:B:444:GLY:HA3	1:B:452:ASN:HD21	1.76	0.50
1:A:366:HIS:HE1	6:A:6818:HOH:O	1.94	0.50
2:C:313:GLN:H	2:C:313:GLN:HE21	1.57	0.50
1:B:414:MET:HE3	1:B:418:ALA:HB3	1.93	0.50
1:A:430:ASN:ND2	6:A:6680:HOH:O	2.31	0.50
5:C:6021:GOL:H2	6:C:6125:HOH:O	2.11	0.50
2:F:352:ARG:HH11	2:F:352:ARG:CG	2.05	0.50
1:B:338:CYS:HB3	1:B:364[B]:CYS:SG	2.51	0.50
2:F:66:GLN:NE2	6:F:6662:HOH:O	2.42	0.50
1:A:62[A]:LYS:HA	5:A:6013:GOL:H31	1.93	0.50
1:A:62[B]:LYS:HA	5:A:6013:GOL:H31	1.93	0.50
1:A:631:PHE:CG	1:A:632:PRO:HA	2.47	0.50
1:B:631:PHE:CG	1:B:632:PRO:HA	2.46	0.50
2:F:265:LYS:HE2	5:F:6001:GOL:H2	1.94	0.50
1:A:160:TYR:CD2	1:A:558:LEU:HD21	2.47	0.49
1:B:430:ASN:ND2	6:B:6693:HOH:O	2.37	0.49
1:A:527:ASN:HD22	1:A:527:ASN:C	2.16	0.49
2:F:338:CYS:CB	2:F:364[B]:CYS:HG	2.25	0.49
2:F:670:ARG:C	2:F:672:VAL:H	2.15	0.49
2:D:631:PHE:CG	2:D:632:PRO:HA	2.47	0.49
1:A:527:ASN:HD21	1:A:529:ASN:HB2	1.76	0.49
2:E:21:PRO:HG3	2:E:77:ARG:CZ	2.43	0.49
2:F:18:PRO:N	6:F:6332:HOH:O	2.44	0.49
1:B:222:ASN:HB3	1:B:227:HIS:CG	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:51:PHE:O	5:F:6003:GOL:H11	2.13	0.49
1:B:338:CYS:SG	1:B:364[B]:CYS:SG	3.11	0.49
2:D:527:ASN:ND2	2:D:529:ASN:H	2.10	0.49
2:F:631:PHE:CG	2:F:632:PRO:HA	2.48	0.49
1:B:527:ASN:ND2	1:B:529:ASN:H	2.10	0.49
2:E:404:ASN:HD21	2:E:405[B]:TPQ:C4	2.26	0.48
2:F:506:LYS:HD2	6:F:6524:HOH:O	2.12	0.48
2:C:338:CYS:HG	2:C:364[B]:CYS:HB3	1.75	0.48
2:F:405[B]:TPQ:H6	2:F:426:THR:O	2.14	0.48
2:C:414[A]:MET:SD	2:C:420:ARG:NH1	2.86	0.48
2:D:313:GLN:H	2:D:313:GLN:NE2	2.12	0.48
2:C:222:ASN:HB3	2:C:227:HIS:CG	2.48	0.48
5:D:6028:GOL:C1	6:D:6662:HOH:O	2.51	0.48
2:C:631:PHE:CG	2:C:632:PRO:HA	2.48	0.48
1:B:338:CYS:CB	1:B:364[B]:CYS:SG	3.02	0.48
2:D:222:ASN:HB3	2:D:227:HIS:CG	2.49	0.48
2:E:160:TYR:CD2	2:E:558:LEU:HD21	2.48	0.48
2:E:157[A]:THR:CG2	2:E:322:GLU:HB3	2.40	0.47
6:C:6858:HOH:O	2:D:286:HIS:HD2	1.98	0.47
1:B:527:ASN:HD21	1:B:529:ASN:HB2	1.79	0.47
2:C:527:ASN:ND2	2:C:529:ASN:H	2.11	0.47
2:E:444:GLY:HA3	2:E:452:ASN:HD21	1.79	0.47
1:B:303:VAL:HG23	6:B:6661:HOH:O	2.13	0.47
5:A:6017:GOL:H32	6:A:6844:HOH:O	2.15	0.47
1:A:333:SER:O	1:A:336:CYS:HB2	2.14	0.47
2:E:425:LEU:HB3	6:E:6515:HOH:O	2.13	0.47
1:A:303:VAL:HG23	6:A:6619:HOH:O	2.15	0.47
2:D:20:ARG:CG	5:D:6028:GOL:H32	2.43	0.47
2:E:424:ARG:HD2	6:E:6067:HOH:O	2.14	0.47
2:D:52:ASN:HD21	2:D:115:ILE:HG22	1.80	0.47
2:E:338:CYS:SG	2:E:342:ILE:CG1	2.93	0.47
2:D:457:GLN:HE22	2:D:552:LEU:H	1.63	0.47
2:E:157[B]:THR:HG22	2:E:323:TYR:OH	2.15	0.47
1:A:390:ARG:HG3	1:A:660:SER:OG	2.15	0.47
2:D:303:VAL:HG23	6:D:6692:HOH:O	2.15	0.47
2:D:663[B]:MET:SD	2:D:667:GLU:HB3	2.55	0.46
2:D:68:LYS:NZ	6:D:6670:HOH:O	2.48	0.46
1:A:313:GLN:NE2	1:A:313:GLN:H	2.13	0.46
2:F:286:HIS:HE1	6:F:6086:HOH:O	1.98	0.46
2:F:338:CYS:HG	2:F:364[B]:CYS:HB3	1.76	0.46
2:D:331:PRO:HD2	6:D:6657:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:468:ILE:H	2:C:473:ASN:ND2	2.08	0.46
2:C:412:VAL:HB	2:C:420:ARG:HB3	1.97	0.46
2:C:106:THR:OG1	6:C:6522:HOH:O	2.12	0.46
2:D:305:TYR:CD2	2:D:456:HIS:HB3	2.51	0.46
1:A:222:ASN:HB3	1:A:227:HIS:CG	2.51	0.46
1:B:62:LYS:NZ	1:B:66:GLN:HE22	2.13	0.45
2:F:335:GLY:O	2:F:336[B]:CYS:SG	2.74	0.45
2:F:352:ARG:NH1	2:F:352:ARG:CG	2.70	0.45
2:F:21:PRO:HG3	2:F:77:ARG:CZ	2.46	0.45
2:C:444:GLY:HA3	2:C:452:ASN:HD21	1.82	0.45
2:F:222:ASN:HB3	2:F:227:HIS:CG	2.51	0.45
1:B:471:ASP:OD1	6:B:6478:HOH:O	2.21	0.45
2:E:631:PHE:CG	2:E:632:PRO:HA	2.51	0.45
2:E:218:HIS:CD2	5:E:6015:GOL:H31	2.50	0.44
1:A:634:SME:HE2	1:A:634:SME:HB3	1.80	0.44
2:F:468:ILE:N	2:F:473:ASN:HD21	2.05	0.44
2:C:405[B]:TPQ:H6	2:C:426:THR:O	2.17	0.44
1:B:313:GLN:NE2	1:B:313:GLN:H	2.13	0.44
2:D:468:ILE:H	2:D:473:ASN:ND2	2.12	0.44
2:C:527:ASN:HD21	2:C:529:ASN:HB2	1.82	0.44
2:C:313:GLN:H	2:C:313:GLN:NE2	2.15	0.44
1:B:120:ASP:OD2	1:B:352:ARG:NH1	2.47	0.44
1:A:308:PRO:HB3	1:B:497:ALA:HB2	2.00	0.44
2:D:405[B]:TPQ:H6	2:D:426:THR:O	2.17	0.44
1:A:310:PHE:CE1	5:A:6017:GOL:H31	2.52	0.44
1:A:342:ILE:CG2	1:A:364:CYS:HB2	2.47	0.44
2:F:436:ASP:H	5:F:6006:GOL:H32	1.83	0.44
2:F:338:CYS:CB	2:F:364[B]:CYS:SG	3.05	0.43
1:B:305:TYR:OH	1:B:405:TPQ:O4	2.24	0.43
1:A:219:LYS:HG3	5:A:6018:GOL:H12	2.00	0.43
2:E:405[A]:TPQ:H6	2:E:426:THR:O	2.18	0.43
1:A:62[B]:LYS:NZ	1:A:66:GLN:OE1	2.28	0.43
1:A:122:CYS:SG	6:A:6724:HOH:O	2.61	0.43
2:D:425[B]:LEU:HD21	2:D:458:HIS:CE1	2.54	0.43
2:D:244[A]:VAL:HG13	6:D:6618:HOH:O	2.17	0.43
1:B:631:PHE:CD1	1:B:632:PRO:HA	2.54	0.43
2:F:117:THR:HG21	5:F:6003:GOL:H12	2.00	0.43
2:E:18:PRO:N	6:E:6405:HOH:O	2.52	0.42
1:B:332:LEU:HB2	1:B:361:ASN:O	2.19	0.42
2:F:23:HIS:CD2	2:F:25:LEU:H	2.19	0.42
1:B:338:CYS:HB3	1:B:364[B]:CYS:HG	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:444:GLY:HA3	2:D:452:ASN:HD21	1.83	0.42
2:C:382:ASN:ND2	6:C:6801:HOH:O	2.52	0.42
2:F:66:GLN:NE2	6:F:6708:HOH:O	2.52	0.42
2:E:427:GLY:O	2:E:634[A]:MET:HG2	2.19	0.42
2:C:157[A]:THR:HG22	2:C:159:GLY:H	1.85	0.42
2:F:252:PHE:HB2	2:F:259:MET:SD	2.58	0.42
2:E:404:ASN:C	2:E:405[A]:TPQ:CA	2.77	0.42
1:A:497:ALA:HB2	1:B:308:PRO:HB3	1.99	0.42
2:C:202:LYS:NZ	6:C:6536:HOH:O	2.51	0.42
1:A:631:PHE:CD1	1:A:632:PRO:HA	2.55	0.42
2:E:118:VAL:HG13	6:E:6026:HOH:O	2.19	0.42
2:C:157[B]:THR:CA	6:C:6628:HOH:O	2.67	0.42
1:B:218:HIS:HD2	1:B:450:ASN:HD22	1.66	0.42
2:C:308:PRO:HB3	2:D:497:ALA:HB2	2.01	0.42
2:C:369:ASP:OD2	2:C:390[A]:ARG:NH1	2.52	0.41
2:C:390[A]:ARG:HH21	2:D:337:ASP:HA	1.85	0.41
2:E:452:ASN:C	2:E:452:ASN:HD22	2.24	0.41
1:A:342:ILE:HG21	1:A:364:CYS:HB2	2.01	0.41
2:E:50:SER:HB2	2:E:352:ARG:CG	2.48	0.41
1:B:452:ASN:HD22	1:B:453:ALA:N	2.18	0.41
1:A:348:HIS:HE1	6:A:6232:HOH:O	2.02	0.41
1:A:414:MET:HE3	1:A:418:ALA:HB3	2.02	0.41
2:D:634[A]:MET:HA	2:D:635:PRO:HD3	1.98	0.41
2:F:136:GLU:OE1	6:F:6497:HOH:O	2.22	0.41
1:A:444:GLY:HA3	1:A:452:ASN:HD21	1.86	0.41
2:D:427:GLY:O	2:D:634[A]:MET:HG2	2.20	0.41
1:A:219:LYS:HB2	5:A:6018:GOL:H32	2.03	0.41
1:A:374:PHE:CD1	1:B:633:LEU:HD13	2.56	0.41
2:D:631:PHE:CD1	2:D:632:PRO:HA	2.56	0.41
1:B:219:LYS:HB2	5:B:6026:GOL:H11	2.02	0.41
2:D:74:LEU:CD2	5:D:6028:GOL:H12	2.47	0.41
2:D:527:ASN:HD21	2:D:529:ASN:HD22	1.69	0.41
2:E:407:TYR:CD2	2:E:425:LEU:HD22	2.55	0.40
2:C:252:PHE:HB2	2:C:259:MET:SD	2.61	0.40
2:C:301:MET:O	2:C:318:LEU:HA	2.21	0.40
2:D:670:ARG:NH2	6:D:6789:HOH:O	2.52	0.40
2:E:157[B]:THR:CB	6:E:6598:HOH:O	2.51	0.40
1:B:452:ASN:HD22	1:B:452:ASN:C	2.23	0.40
1:A:632:PRO:HD2	1:B:655:LEU:HD11	2.02	0.40
2:C:120:ASP:HA	2:C:352:ARG:NH2	2.36	0.40
1:B:390:ARG:HG3	1:B:660:SER:OG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:575:TYR:O	2:E:576:LYS:HD2	2.21	0.40
2:E:303:VAL:HG23	6:E:6510:HOH:O	2.21	0.40
2:C:66:GLN:NE2	6:C:6757:HOH:O	2.54	0.40
2:E:645:PRO:O	2:E:646:ARG:HD2	2.21	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	664/660 (101%)	642 (97%)	21 (3%)	1 (0%)	52 32
1	B	661/660 (100%)	643 (97%)	17 (3%)	1 (0%)	52 32
2	C	668/660 (101%)	649 (97%)	19 (3%)	0	100 100
2	D	665/660 (101%)	644 (97%)	21 (3%)	0	100 100
2	E	660/660 (100%)	639 (97%)	21 (3%)	0	100 100
2	F	661/660 (100%)	640 (97%)	21 (3%)	0	100 100
All	All	3979/3960 (100%)	3857 (97%)	120 (3%)	2 (0%)	56 35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	333	SER
1	A	333	SER

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	577/565 (102%)	564 (98%)	13 (2%)	58	37
1	B	574/565 (102%)	560 (98%)	14 (2%)	57	36
2	C	581/566 (103%)	570 (98%)	11 (2%)	65	46
2	D	578/566 (102%)	562 (97%)	16 (3%)	51	29
2	E	573/566 (101%)	563 (98%)	10 (2%)	68	51
2	F	574/566 (101%)	564 (98%)	10 (2%)	68	51
All	All	3457/3394 (102%)	3383 (98%)	74 (2%)	61	42

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LYS
1	A	84	LEU
1	A	146	ASN
1	A	157[A]	THR
1	A	157[B]	THR
1	A	202	LYS
1	A	313	GLN
1	A	329	THR
1	A	334	LEU
1	A	394	LEU
1	A	452	ASN
1	A	527	ASN
1	A	641	LEU
1	B	47	LYS
1	B	84	LEU
1	B	109	LEU
1	B	313	GLN
1	B	329	THR
1	B	332	LEU
1	B	359	VAL
1	B	421	LEU
1	B	452	ASN
1	B	481	LYS
1	B	527	ASN
1	B	576	LYS
1	B	633	LEU
1	B	672	VAL

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Mol	Chain	Res	Type
2	C	68	LYS
2	C	84	LEU
2	C	140	LEU
2	C	313	GLN
2	C	329	THR
2	C	360	LYS
2	C	390[A]	ARG
2	C	390[B]	ARG
2	C	421	LEU
2	C	452	ASN
2	C	527	ASN
2	D	84	LEU
2	D	109	LEU
2	D	140	LEU
2	D	146	ASN
2	D	213	ARG
2	D	244[A]	VAL
2	D	244[B]	VAL
2	D	313	GLN
2	D	329	THR
2	D	339	LYS
2	D	342	ILE
2	D	394	LEU
2	D	452	ASN
2	D	506	LYS
2	D	527	ASN
2	D	554	LYS
2	E	109	LEU
2	E	118	VAL
2	E	146	ASN
2	E	201	LYS
2	E	213	ARG
2	E	329	THR
2	E	342	ILE
2	E	394	LEU
2	E	452	ASN
2	E	554	LYS
2	F	84	LEU
2	F	140	LEU
2	F	313	GLN
2	F	329	THR
2	F	336[A]	CYS

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Mol	Chain	Res	Type
2	F	336[B]	CYS
2	F	352	ARG
2	F	452	ASN
2	F	554	LYS
2	F	558	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	146	ASN
1	A	313	GLN
1	A	348	HIS
1	A	361	ASN
1	A	366	HIS
1	A	382	ASN
1	A	452	ASN
1	A	527	ASN
1	B	66	GLN
1	B	288	ASN
1	B	313	GLN
1	B	348	HIS
1	B	361	ASN
1	B	450	ASN
1	B	452	ASN
1	B	527	ASN
2	C	288	ASN
2	C	313	GLN
2	C	361	ASN
2	C	382	ASN
2	C	452	ASN
2	C	473	ASN
2	C	527	ASN
2	C	547	GLN
2	D	52	ASN
2	D	146	ASN
2	D	313	GLN
2	D	452	ASN
2	D	457	GLN
2	D	473	ASN
2	D	527	ASN
2	E	23	HIS

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Mol	Chain	Res	Type
2	E	146	ASN
2	E	218	HIS
2	E	286	HIS
2	E	294	HIS
2	E	348	HIS
2	E	361	ASN
2	E	430	ASN
2	E	452	ASN
2	F	23	HIS
2	F	66	GLN
2	F	70	GLN
2	F	286	HIS
2	F	313	GLN
2	F	361	ASN
2	F	382	ASN
2	F	452	ASN
2	F	473	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	TPQ	A	405	1	13,14,15	2.04	3 (23%)	15,19,21	2.27	4 (26%)
1	SME	A	634	1	7,8,9	5.00	1 (14%)	6,9,11	3.50	2 (33%)
1	TPQ	B	405	1	13,14,15	2.12	4 (30%)	15,19,21	2.23	4 (26%)
1	SME	B	634	1	7,8,9	4.90	1 (14%)	6,9,11	3.18	2 (33%)
2	TPQ	C	405[A]	-	13,14,15	2.08	5 (38%)	15,19,21	2.23	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	TPQ	C	405[B]	3	13,14,15	2.19	4 (30%)	15,19,21	1.78	2 (13%)
2	TPQ	D	405[A]	-	13,14,15	2.11	4 (30%)	15,19,21	2.12	5 (33%)
2	TPQ	D	405[B]	3	13,14,15	2.16	4 (30%)	15,19,21	2.10	3 (20%)
2	TPQ	E	405[A]	3	13,14,15	2.20	4 (30%)	15,19,21	1.71	3 (20%)
2	TPQ	E	405[B]	-	13,14,15	2.12	5 (38%)	15,19,21	2.10	3 (20%)
2	TPQ	F	405[A]	-	13,14,15	1.97	3 (23%)	15,19,21	2.46	4 (26%)
2	TPQ	F	405[B]	-	13,14,15	2.22	4 (30%)	15,19,21	1.77	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPQ	A	405	1	-	0/4/22/24	0/1/1/1
1	SME	A	634	1	-	0/5/7/9	0/0/0/0
1	TPQ	B	405	1	-	0/4/22/24	0/1/1/1
1	SME	B	634	1	-	0/5/7/9	0/0/0/0
2	TPQ	C	405[A]	-	-	0/4/22/24	0/1/1/1
2	TPQ	C	405[B]	3	-	0/4/22/24	0/1/1/1
2	TPQ	D	405[A]	-	-	0/4/22/24	0/1/1/1
2	TPQ	D	405[B]	3	-	0/4/22/24	0/1/1/1
2	TPQ	E	405[A]	3	-	0/4/22/24	0/1/1/1
2	TPQ	E	405[B]	-	-	0/4/22/24	0/1/1/1
2	TPQ	F	405[A]	-	-	0/4/22/24	0/1/1/1
2	TPQ	F	405[B]	-	-	0/4/22/24	0/1/1/1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	405[A]	TPQ	C6-C5	-2.14	1.38	1.44
2	F	405[A]	TPQ	C6-C5	-2.10	1.38	1.44
2	E	405[B]	TPQ	C6-C5	-2.09	1.38	1.44
2	C	405[A]	TPQ	C6-C5	-2.04	1.38	1.44
1	B	405	TPQ	C6-C1	2.02	1.39	1.34
2	C	405[A]	TPQ	C6-C1	2.04	1.40	1.34
2	E	405[B]	TPQ	C6-C1	2.04	1.40	1.34
2	D	405[B]	TPQ	C3-C4	2.11	1.39	1.35
2	E	405[A]	TPQ	C3-C4	2.11	1.39	1.35
2	C	405[A]	TPQ	C3-C4	2.13	1.39	1.35
2	E	405[A]	TPQ	C6-C1	2.15	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	405[B]	TPQ	C6-C1	2.15	1.40	1.34
2	C	405[B]	TPQ	C3-C4	2.15	1.39	1.35
2	C	405[B]	TPQ	C6-C1	2.25	1.40	1.34
2	F	405[B]	TPQ	C3-C4	2.26	1.39	1.35
2	F	405[B]	TPQ	C6-C1	2.32	1.40	1.34
2	E	405[B]	TPQ	C3-C4	2.33	1.39	1.35
1	A	405	TPQ	C3-C4	2.37	1.39	1.35
2	D	405[A]	TPQ	C3-C4	2.55	1.39	1.35
1	B	405	TPQ	C3-C4	2.57	1.39	1.35
1	A	405	TPQ	O2-C2	3.98	1.35	1.24
2	F	405[A]	TPQ	O2-C2	3.98	1.35	1.24
2	F	405[A]	TPQ	O5-C5	4.17	1.36	1.24
2	C	405[A]	TPQ	O2-C2	4.18	1.36	1.24
1	B	405	TPQ	O2-C2	4.19	1.36	1.24
2	C	405[B]	TPQ	O2-C2	4.31	1.36	1.24
2	D	405[A]	TPQ	O2-C2	4.35	1.36	1.24
2	D	405[B]	TPQ	O2-C2	4.38	1.36	1.24
2	E	405[B]	TPQ	O2-C2	4.38	1.36	1.24
2	D	405[A]	TPQ	O5-C5	4.39	1.36	1.24
2	E	405[B]	TPQ	O5-C5	4.39	1.36	1.24
1	A	405	TPQ	O5-C5	4.41	1.36	1.24
2	F	405[B]	TPQ	O2-C2	4.42	1.36	1.24
2	E	405[A]	TPQ	O2-C2	4.48	1.36	1.24
2	C	405[A]	TPQ	O5-C5	4.48	1.37	1.24
1	B	405	TPQ	O5-C5	4.56	1.37	1.24
2	D	405[B]	TPQ	O5-C5	4.66	1.37	1.24
2	E	405[A]	TPQ	O5-C5	4.73	1.37	1.24
2	F	405[B]	TPQ	O5-C5	4.78	1.37	1.24
2	C	405[B]	TPQ	O5-C5	4.86	1.38	1.24
1	B	634	SME	OE-S	12.87	1.81	1.51
1	A	634	SME	OE-S	13.17	1.82	1.51

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	405[A]	TPQ	C1-C6-C5	-6.71	118.88	122.97
1	B	405	TPQ	C1-C6-C5	-6.15	119.22	122.97
2	C	405[A]	TPQ	C1-C6-C5	-6.08	119.27	122.97
1	A	405	TPQ	C1-C6-C5	-6.03	119.30	122.97
2	D	405[B]	TPQ	C1-C6-C5	-5.84	119.41	122.97
2	E	405[B]	TPQ	C1-C6-C5	-5.42	119.67	122.97
2	D	405[A]	TPQ	C1-C6-C5	-5.30	119.74	122.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	405[B]	TPQ	C1-C6-C5	-4.74	120.08	122.97
2	C	405[B]	TPQ	C1-C6-C5	-4.45	120.26	122.97
2	E	405[A]	TPQ	C1-C6-C5	-4.12	120.46	122.97
2	E	405[B]	TPQ	O-C-CA	-4.00	115.06	125.49
2	F	405[A]	TPQ	O-C-CA	-3.93	115.25	125.49
2	C	405[A]	TPQ	O-C-CA	-3.93	115.26	125.49
2	D	405[A]	TPQ	O-C-CA	-3.44	116.53	125.49
1	A	405	TPQ	O-C-CA	-3.40	116.64	125.49
1	B	405	TPQ	O-C-CA	-3.01	117.65	125.49
2	E	405[A]	TPQ	O-C-CA	-2.26	119.61	125.49
2	D	405[A]	TPQ	O2-C2-C1	-2.19	118.94	120.85
1	B	634	SME	O-C-CA	-2.13	119.95	125.49
1	A	634	SME	O-C-CA	-2.06	120.13	125.49
2	D	405[A]	TPQ	C3-C2-C1	2.17	119.92	118.30
2	C	405[A]	TPQ	C3-C2-C1	2.18	119.94	118.30
2	D	405[B]	TPQ	C3-C2-C1	2.25	119.98	118.30
2	F	405[A]	TPQ	C3-C2-C1	2.50	120.17	118.30
1	A	405	TPQ	C6-C1-C2	2.56	120.25	118.44
1	B	405	TPQ	C3-C2-C1	2.66	120.29	118.30
1	B	405	TPQ	C6-C1-C2	3.19	120.69	118.44
2	E	405[A]	TPQ	C6-C1-C2	3.23	120.72	118.44
2	D	405[A]	TPQ	C6-C1-C2	3.28	120.75	118.44
2	E	405[B]	TPQ	C6-C1-C2	3.33	120.79	118.44
2	C	405[A]	TPQ	C6-C1-C2	3.34	120.80	118.44
2	F	405[B]	TPQ	C6-C1-C2	3.37	120.82	118.44
1	A	405	TPQ	C3-C2-C1	3.40	120.84	118.30
2	C	405[B]	TPQ	C6-C1-C2	3.48	120.90	118.44
2	D	405[B]	TPQ	C6-C1-C2	3.64	121.01	118.44
2	F	405[A]	TPQ	C6-C1-C2	3.83	121.14	118.44
1	B	634	SME	OE-S-CE	7.49	118.81	106.41
1	A	634	SME	OE-S-CE	8.16	119.93	106.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	405	TPQ	1	0
1	A	634	SME	1	0
1	B	405	TPQ	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	634	SME	1	0
2	C	405[A]	TPQ	1	0
2	C	405[B]	TPQ	1	0
2	D	405[A]	TPQ	1	0
2	D	405[B]	TPQ	4	0
2	E	405[A]	TPQ	4	0
2	E	405[B]	TPQ	3	0
2	F	405[A]	TPQ	1	0
2	F	405[B]	TPQ	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 6 are monoatomic - leaving 30 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	$\#\|Z\| > 2$
5	GOL	A	6005	-	5,5,5	0.36	0	5,5,5	0.17	0
5	GOL	A	6012	-	5,5,5	0.27	0	5,5,5	0.46	0
5	GOL	A	6013	-	5,5,5	0.31	0	5,5,5	0.39	0
5	GOL	A	6017	-	5,5,5	0.34	0	5,5,5	0.33	0
5	GOL	A	6018	-	5,5,5	0.30	0	5,5,5	0.20	0
5	GOL	A	6027	-	5,5,5	0.28	0	5,5,5	0.44	0
5	GOL	B	6004	-	5,5,5	0.24	0	5,5,5	0.21	0
5	GOL	B	6009	-	5,5,5	0.26	0	5,5,5	0.45	0
5	GOL	B	6023	-	5,5,5	0.40	0	5,5,5	0.17	0
5	GOL	B	6024	-	5,5,5	0.37	0	5,5,5	0.45	0
5	GOL	B	6025	-	5,5,5	0.30	0	5,5,5	0.40	0
5	GOL	B	6026	-	5,5,5	0.43	0	5,5,5	0.27	0
5	GOL	C	6002	-	5,5,5	0.31	0	5,5,5	0.51	0
5	GOL	C	6007	-	5,5,5	0.28	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	PO4	C	6010	-	4,4,4	0.42	0	6,6,6	0.28	0
5	GOL	C	6021	-	5,5,5	0.44	0	5,5,5	0.53	0
5	GOL	C	6029	-	5,5,5	0.35	0	5,5,5	0.25	0
5	GOL	D	6028	-	5,5,5	0.52	0	5,5,5	0.55	0
5	GOL	D	6030	-	5,5,5	0.27	0	5,5,5	0.64	0
5	GOL	E	6014	-	5,5,5	0.33	0	5,5,5	0.19	0
5	GOL	E	6015	-	5,5,5	0.44	0	5,5,5	0.12	0
5	GOL	E	6016	-	5,5,5	0.38	0	5,5,5	0.30	0
5	GOL	E	6019	-	5,5,5	0.29	0	5,5,5	0.39	0
5	GOL	E	6020	-	5,5,5	0.32	0	5,5,5	0.20	0
5	GOL	E	6022	-	5,5,5	0.36	0	5,5,5	0.36	0
5	GOL	F	6001	-	5,5,5	0.36	0	5,5,5	0.29	0
5	GOL	F	6003	-	5,5,5	0.35	0	5,5,5	0.64	0
5	GOL	F	6006	-	5,5,5	0.34	0	5,5,5	0.20	0
5	GOL	F	6008	-	5,5,5	0.26	0	5,5,5	0.34	0
4	PO4	F	6011	-	4,4,4	0.43	0	6,6,6	0.26	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
5	GOL	A	6005	-	-	0/4/4/4	0/0/0/0
5	GOL	A	6012	-	-	0/4/4/4	0/0/0/0
5	GOL	A	6013	-	-	0/4/4/4	0/0/0/0
5	GOL	A	6017	-	-	0/4/4/4	0/0/0/0
5	GOL	A	6018	-	-	0/4/4/4	0/0/0/0
5	GOL	A	6027	-	-	0/4/4/4	0/0/0/0
5	GOL	B	6004	-	-	0/4/4/4	0/0/0/0
5	GOL	B	6009	-	-	0/4/4/4	0/0/0/0
5	GOL	B	6023	-	-	0/4/4/4	0/0/0/0
5	GOL	B	6024	-	-	0/4/4/4	0/0/0/0
5	GOL	B	6025	-	-	0/4/4/4	0/0/0/0
5	GOL	B	6026	-	-	0/4/4/4	0/0/0/0
5	GOL	C	6002	-	-	0/4/4/4	0/0/0/0
5	GOL	C	6007	-	-	0/4/4/4	0/0/0/0
4	PO4	C	6010	-	-	0/0/0/0	0/0/0/0
5	GOL	C	6021	-	-	0/4/4/4	0/0/0/0
5	GOL	C	6029	-	-	0/4/4/4	0/0/0/0
5	GOL	D	6028	-	-	0/4/4/4	0/0/0/0
5	GOL	D	6030	-	-	0/4/4/4	0/0/0/0
5	GOL	E	6014	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	E	6015	-	-	0/4/4/4	0/0/0/0
5	GOL	E	6016	-	-	0/4/4/4	0/0/0/0
5	GOL	E	6019	-	-	0/4/4/4	0/0/0/0
5	GOL	E	6020	-	-	0/4/4/4	0/0/0/0
5	GOL	E	6022	-	-	0/4/4/4	0/0/0/0
5	GOL	F	6001	-	-	0/4/4/4	0/0/0/0
5	GOL	F	6003	-	-	0/4/4/4	0/0/0/0
5	GOL	F	6006	-	-	0/4/4/4	0/0/0/0
5	GOL	F	6008	-	-	0/4/4/4	0/0/0/0
4	PO4	F	6011	-	-	0/0/0/0	0/0/0/0

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.

11 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	6013	GOL	2	0
5	A	6017	GOL	2	0
5	A	6018	GOL	2	0
5	B	6023	GOL	1	0
5	B	6026	GOL	1	0
5	C	6021	GOL	2	0
5	D	6028	GOL	9	0
5	E	6015	GOL	2	0
5	F	6001	GOL	1	0
5	F	6003	GOL	2	0
5	F	6006	GOL	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	653/660 (98%)	-0.25	14 (2%)	67	71	14, 19, 31, 55	0
1	B	653/660 (98%)	-0.24	15 (2%)	64	68	14, 19, 31, 55	0
2	C	654/660 (99%)	-0.18	13 (1%)	68	73	14, 19, 32, 48	0
2	D	654/660 (99%)	-0.28	14 (2%)	67	71	14, 19, 29, 51	0
2	E	654/660 (99%)	-0.28	12 (1%)	71	76	13, 19, 29, 50	0
2	F	654/660 (99%)	-0.19	11 (1%)	73	77	13, 19, 32, 49	0
All	All	3922/3960 (99%)	-0.24	79 (2%)	68	73	13, 19, 31, 55	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	334	LEU	15.2
2	E	672	VAL	10.7
2	F	672	VAL	10.5
2	F	334	LEU	10.2
2	D	672	VAL	9.7
2	C	672	VAL	8.3
1	B	672	VAL	8.0
1	A	672	VAL	7.8
2	F	335	GLY	6.3
2	D	22	ALA	6.2
1	A	334	LEU	5.8
1	B	671	ALA	5.7
1	B	22	ALA	5.5
2	D	18	PRO	5.5
1	A	671	ALA	5.3
1	B	334	LEU	5.3
2	E	18	PRO	5.2
2	E	22	ALA	5.2
1	B	18	PRO	5.0

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Mol	Chain	Res	Type	RSRZ
2	D	19	ALA	4.9
2	C	335	GLY	4.8
1	A	22	ALA	4.8
2	E	19	ALA	4.7
2	F	336[A]	CYS	4.3
1	A	18	PRO	4.2
1	B	19	ALA	4.2
1	A	333	SER	4.1
2	C	333	SER	4.1
2	E	46	GLY	4.0
2	D	20	ARG	4.0
1	A	19	ALA	3.7
1	A	335	GLY	3.7
2	E	20	ARG	3.7
2	F	333	SER	3.6
2	F	46	GLY	3.4
2	C	46	GLY	3.4
2	D	437[A]	ASP	3.4
2	D	46	GLY	3.4
2	D	210	ASN	3.3
1	A	670	ARG	3.2
1	A	332	LEU	3.1
1	B	335	GLY	3.1
2	E	671	ALA	3.1
1	A	437[A]	ASP	3.0
2	D	671	ALA	3.0
2	C	437	ASP	2.9
2	E	210	ASN	2.9
2	F	210	ASN	2.9
2	D	45	ALA	2.9
1	B	670	ARG	2.9
2	D	670	ARG	2.9
2	C	210	ASN	2.9
1	B	437	ASP	2.8
2	C	45	ALA	2.8
1	A	20	ARG	2.8
1	A	230	GLU	2.7
2	E	45	ALA	2.7
2	F	437	ASP	2.7
2	E	437[A]	ASP	2.7
2	F	87	GLY	2.6
2	F	45	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	48	LYS	2.6
1	B	20	ARG	2.6
2	D	211	ARG	2.5
2	C	87	GLY	2.5
1	B	230	GLU	2.4
2	F	670	ARG	2.4
2	E	670	ARG	2.3
2	D	48	LYS	2.3
2	C	230	GLU	2.3
1	B	122	CYS	2.3
2	C	670	ARG	2.2
2	D	244[A]	VAL	2.2
1	B	121	LEU	2.2
1	B	332	LEU	2.2
2	C	86	ALA	2.2
2	E	48	LYS	2.1
1	A	121	LEU	2.1
1	B	669	LYS	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	TPQ	C	405[A]	14/15	0.88	0.26	-	18,22,23,24	11
2	TPQ	E	405[B]	14/15	0.89	0.22	-	18,21,22,23	11
2	TPQ	F	405[B]	14/15	0.89	0.24	-	18,20,22,23	11
2	TPQ	C	405[B]	14/15	0.88	0.26	-	18,18,19,20	11
1	TPQ	B	405	14/15	0.89	0.15	-	21,28,30,31	1
2	TPQ	E	405[A]	14/15	0.89	0.22	-	18,20,21,21	11
1	SME	B	634	9/10	0.92	0.14	-	19,20,26,30	1
1	SME	A	634	9/10	0.90	0.13	-	18,19,32,32	0
1	TPQ	A	405	14/15	0.89	0.15	-	22,29,30,31	1
2	TPQ	D	405[B]	14/15	0.90	0.21	-	17,19,20,21	11
2	TPQ	D	405[A]	14/15	0.90	0.21	-	17,20,22,23	11
2	TPQ	F	405[A]	14/15	0.89	0.24	-	18,20,23,23	11

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	6021	6/6	0.86	0.28	24.22	35,39,39,42	0
5	GOL	B	6025	6/6	0.60	0.34	20.76	38,42,43,43	0
5	GOL	B	6024	6/6	0.84	0.19	17.15	56,58,59,59	0
5	GOL	E	6016	6/6	0.79	0.20	12.34	57,58,58,59	0
5	GOL	A	6017	6/6	0.83	0.16	11.54	43,45,46,48	0
5	GOL	C	6029	6/6	0.76	0.23	10.42	29,40,41,43	0
5	GOL	A	6027	6/6	0.81	0.16	9.61	48,50,50,52	0
5	GOL	E	6020	6/6	0.68	0.18	5.91	59,59,59,61	0
5	GOL	E	6014	6/6	0.79	0.19	5.62	51,52,53,53	0
5	GOL	E	6022	6/6	0.03	0.51	5.53	68,68,69,69	0
5	GOL	A	6012	6/6	0.81	0.16	5.20	34,37,38,41	0
5	GOL	F	6001	6/6	0.87	0.15	4.89	35,39,40,41	0
5	GOL	E	6015	6/6	0.73	0.21	4.47	50,52,52,53	0
5	GOL	F	6003	6/6	0.68	0.29	4.32	45,46,47,48	0
5	GOL	B	6009	6/6	0.90	0.15	3.89	35,37,39,41	0
5	GOL	F	6008	6/6	0.79	0.14	3.47	40,41,41,41	0
5	GOL	E	6019	6/6	0.82	0.15	2.95	37,39,40,42	0
5	GOL	D	6028	6/6	0.65	0.49	2.93	61,61,61,61	0
5	GOL	B	6023	6/6	0.74	0.23	2.62	54,56,57,57	0
5	GOL	A	6013	6/6	0.75	0.16	2.43	53,55,56,56	0
5	GOL	C	6002	6/6	0.79	0.15	2.38	40,43,44,45	0
5	GOL	F	6006	6/6	0.72	0.15	2.08	42,43,44,45	0
5	GOL	C	6007	6/6	0.81	0.12	2.06	37,39,39,39	0
5	GOL	D	6030	6/6	0.84	0.13	2.00	34,36,37,38	0
5	GOL	B	6004	6/6	0.82	0.14	1.09	48,49,50,52	0
5	GOL	A	6005	6/6	0.68	0.14	0.89	49,50,50,50	0
3	CU	D	801	1/1	1.00	0.04	-2.03	19,19,19,19	0
3	CU	F	801	1/1	1.00	0.05	-3.12	18,18,18,18	0
3	CU	C	801	1/1	1.00	0.05	-3.27	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	PO4	F	6011	5/5	0.89	0.18	-	50,51,52,52	0
3	CU	B	801	1/1	1.00	0.06	-	19,19,19,19	0
5	GOL	A	6018	6/6	0.65	0.21	-	52,52,52,54	0
3	CU	E	801	1/1	1.00	0.04	-	18,18,18,18	0
4	PO4	C	6010	5/5	0.91	0.19	-	50,52,52,53	0
3	CU	A	801	1/1	1.00	0.06	-	19,19,19,19	0
5	GOL	B	6026	6/6	0.83	0.20	-	52,52,53,53	0

6.5 Other polymers

There are no such residues in this entry.