



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:39 PM UTC

PDB ID : 4EV2 / pdb_00004ev2
Title : Crystal structure of copper amine oxidase-1 from Hansenula polymorpha in complex with ethylamine
Authors : Klema, V.J.; Solheid, C.J.; Wilmot, C.M.
Deposited on : 2012-04-25
Resolution : 2.18 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

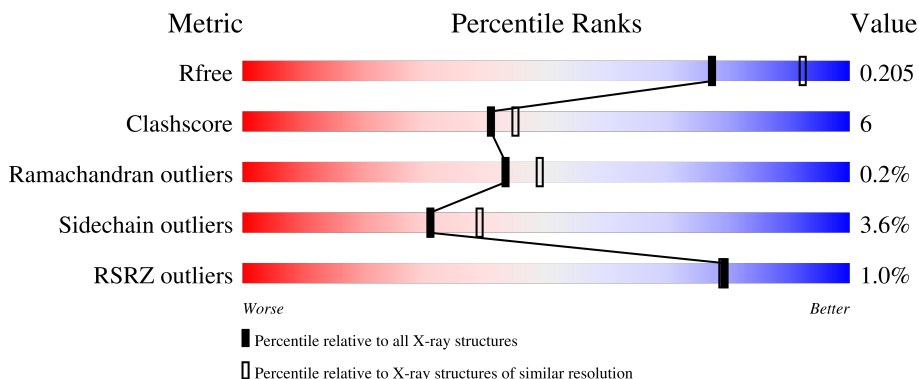
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	692	 84% 10% • 5%
1	B	692	 82% 11% • 5%
1	C	692	 81% 12% • 5%
1	D	692	 84% 9% • 5%
1	E	692	 82% 11% • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	692	 % 84% 10% • 5%

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
1	TYQ	A	405	-	-	X	-
2	GOL	A	703	-	-	X	-
2	GOL	B	701	-	-	X	-
2	GOL	B	707	-	-	X	-
2	GOL	E	704	-	-	X	-
2	GOL	E	705	-	-	X	-
2	GOL	F	702	-	-	X	-
5	NEH	A	708	-	-	X	-

2 Entry composition [i](#)

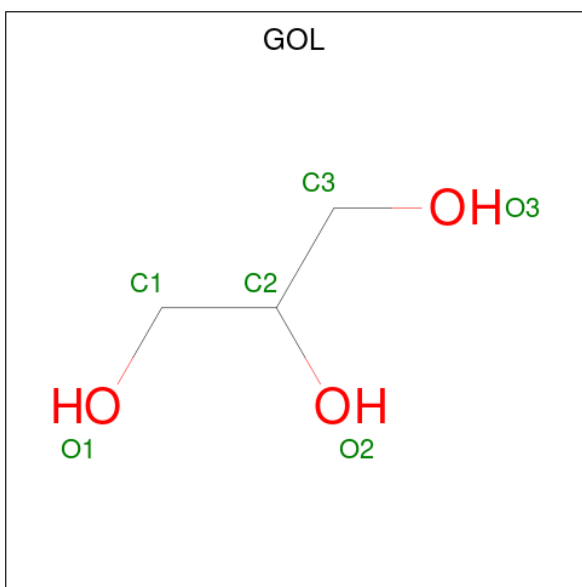
There are 7 unique types of molecules in this entry. The entry contains 35006 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 primary amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	654	Total 5236	C 3339	N 891	O 981	S 25	0	13	0
1	B	655	Total 5238	C 3337	N 896	O 979	S 26	0	11	1
1	C	655	Total 5236	C 3335	N 891	O 983	S 27	0	12	0
1	D	655	Total 5232	C 3333	N 897	O 977	S 25	0	9	0
1	E	654	Total 5268	C 3358	N 900	O 983	S 27	0	18	0
1	F	655	Total 5233	C 3333	N 899	O 976	S 25	0	9	0

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

Continued on next page...

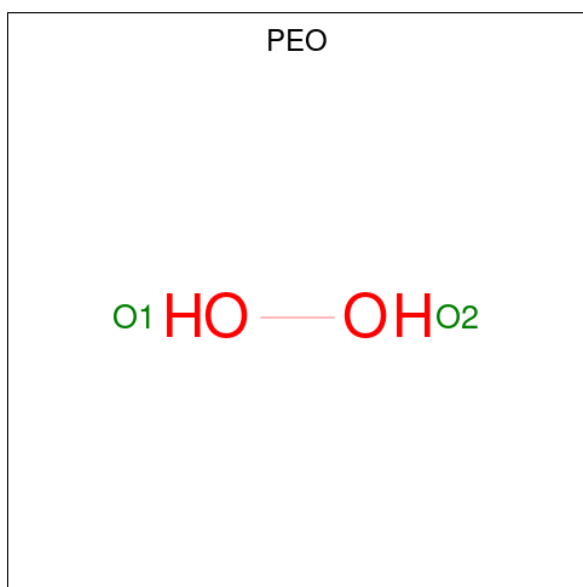
Continued from previous page...

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

- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

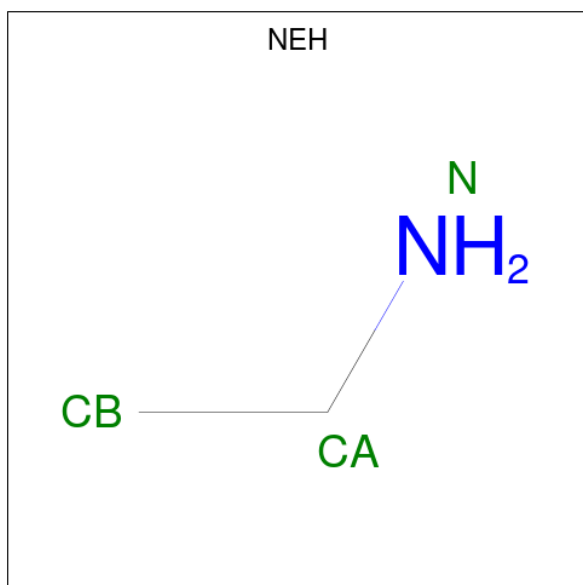
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cu 1 1	0	0
3	B	1	Total Cu 1 1	0	0
3	C	1	Total Cu 1 1	0	0
3	D	1	Total Cu 1 1	0	0
3	E	1	Total Cu 1 1	0	0
3	F	1	Total Cu 1 1	0	0

- Molecule 4 is HYDROGEN PEROXIDE (CCD ID: PEO) (formula: H₂O₂).



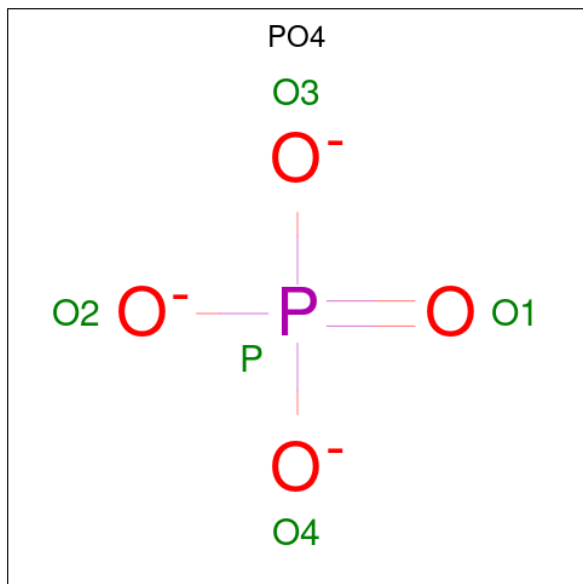
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 2 2	0	0
4	B	1	Total O 2 2	0	0
4	E	1	Total O 2 2	0	0
4	F	1	Total O 2 2	0	0

- Molecule 5 is ETHANAMINE (CCD ID: NEH) (formula: C₂H₇N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			3	2	1		
5	B	1	Total	C	N	0	0
			3	2	1		
5	C	1	Total	C	N	0	0
			3	2	1		
5	D	1	Total	C	N	0	0
			3	2	1		
5	E	1	Total	C	N	0	0
			3	2	1		
5	F	1	Total	C	N	0	0
			3	2	1		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	569	Total	O	0	2
			571	571		
7	B	653	Total	O	0	3
			656	656		
7	C	534	Total	O	0	3
			537	537		

Continued on next page...

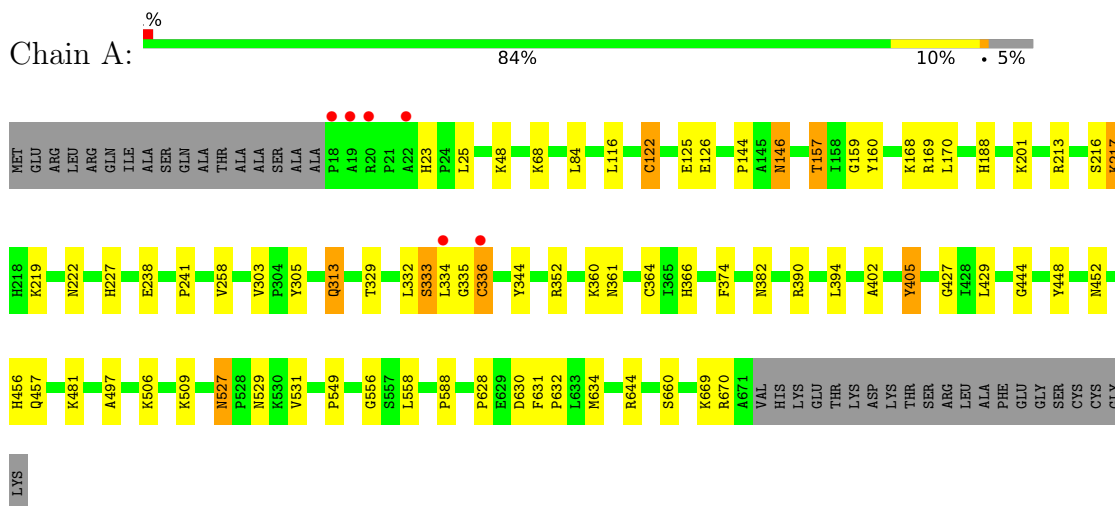
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	496	Total 498	O 498	0	2
7	E	517	Total 519	O 519	0	2
7	F	557	Total 559	O 559	0	2

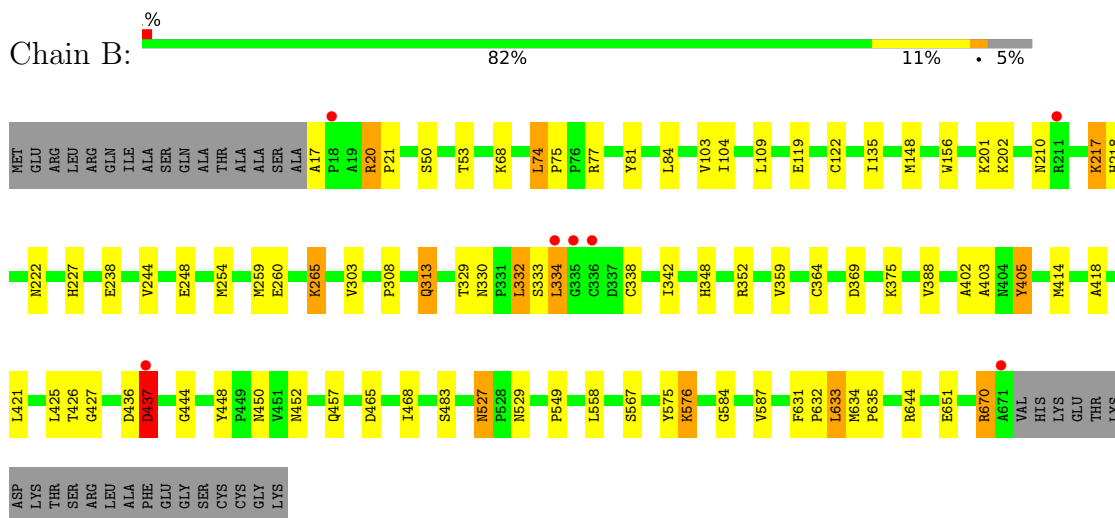
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

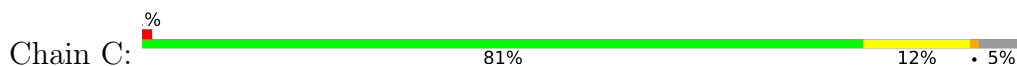
- Molecule 1: Peroxisomal primary amine oxidase



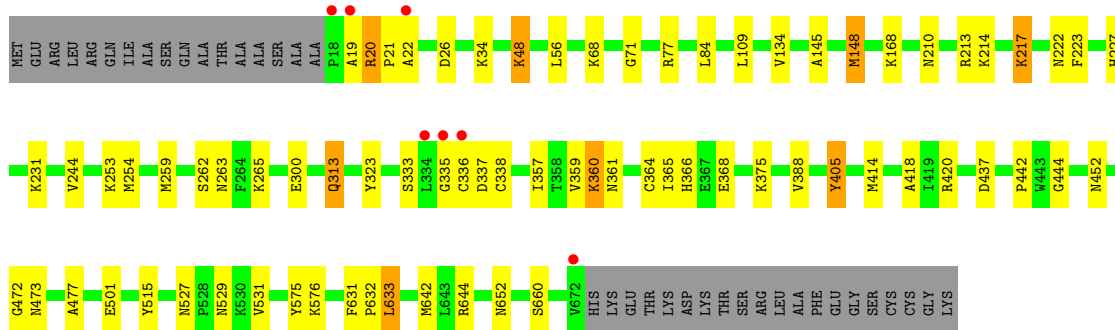
- Molecule 1: Peroxisomal primary amine oxidase



- Molecule 1: Peroxisomal primary amine oxidase



Chain F: %
84% 10% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.41Å 232.83Å 105.12Å 90.00° 96.66° 90.00°	Depositor
Resolution (Å)	48.97 – 2.18 48.97 – 2.18	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.97-2.18) 99.5 (48.97-2.18)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.18Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.150 , 0.201 (Not available) , 0.205	Depositor DCC
R_{free} test set	12996 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtrriage
Anisotropy	0.081	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.014 for l,-k,h	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	35006	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PEO, CU, PO4, GOL, NEH, TYQ

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	0.87	0/5410	0.97	5/7360 (0.1%)
1	B	0.96	0/5407	1.04	20/7355 (0.3%)
1	C	0.88	3/5410 (0.1%)	0.98	10/7362 (0.1%)
1	D	0.81	1/5394 (0.0%)	0.93	4/7338 (0.1%)
1	E	0.90	0/5456	0.95	8/7423 (0.1%)
1	F	0.91	2/5395 (0.0%)	0.98	3/7339 (0.0%)
All	All	0.89	6/32472 (0.0%)	0.98	50/44177 (0.1%)

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	E	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	518	ALA	CA-CB	6.28	1.63	1.53
1	C	122	CYS	CB-SG	5.96	2.00	1.81
1	F	477	ALA	CA-CB	5.32	1.61	1.53
1	C	538	PRO	CA-C	5.32	1.54	1.51
1	C	173	ALA	CA-CB	5.25	1.60	1.53
1	F	134	VAL	CA-CB	5.08	1.60	1.54

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	75	PRO	CA-C-N	-8.54	111.22	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	75	PRO	C-N-CA	-8.54	111.22	119.85
1	B	670	ARG	N-CA-C	8.15	119.79	111.07
1	E	334	LEU	N-CA-C	7.71	124.09	111.37
1	B	549	PRO	CA-C-N	-6.39	113.40	119.85
1	B	549	PRO	C-N-CA	-6.39	113.40	119.85
1	E	337	ASP	N-CA-C	-6.18	104.81	112.90
1	B	587	VAL	CA-C-N	-6.17	113.32	119.93
1	B	587	VAL	C-N-CA	-6.17	113.32	119.93
1	B	104	ILE	N-CA-C	-6.00	107.41	113.47
1	B	437	ASP	N-CA-C	5.96	119.65	112.38
1	B	448	TYR	N-CA-C	-5.94	102.79	108.13
1	B	436	ASP	CA-C-N	5.91	130.05	120.60
1	B	436	ASP	C-N-CA	5.91	130.05	120.60
1	A	336	CYS	N-CA-C	5.89	118.91	108.24
1	C	337	ASP	N-CA-C	-5.75	104.98	112.23
1	E	333	SER	CA-C-N	5.73	129.42	120.82
1	E	333	SER	C-N-CA	5.73	129.42	120.82
1	C	355	ASP	CA-C-N	5.68	125.97	119.83
1	C	355	ASP	C-N-CA	5.68	125.97	119.83
1	B	465	ASP	CA-C-N	-5.68	114.47	120.66
1	B	465	ASP	C-N-CA	-5.68	114.47	120.66
1	E	74	LEU	CA-C-N	5.58	123.68	119.66
1	E	74	LEU	C-N-CA	5.58	123.68	119.66
1	C	62	LYS	N-CA-C	-5.57	105.12	111.14
1	A	549	PRO	CA-C-N	-5.50	114.59	120.03
1	A	549	PRO	C-N-CA	-5.50	114.59	120.03
1	B	210	ASN	N-CA-C	5.48	116.93	111.07
1	C	448	TYR	CA-C-N	-5.45	114.15	119.76
1	C	448	TYR	C-N-CA	-5.45	114.15	119.76
1	C	175	VAL	N-CA-C	5.42	117.11	108.87
1	E	448	TYR	CA-C-N	-5.38	114.39	119.76
1	E	448	TYR	C-N-CA	-5.38	114.39	119.76
1	D	276	ILE	N-CA-C	5.36	116.61	109.37
1	A	448	TYR	CA-C-N	-5.29	114.12	119.83
1	A	448	TYR	C-N-CA	-5.29	114.12	119.83
1	D	143	ILE	CB-CA-C	5.25	116.34	110.52
1	F	145	ALA	N-CA-C	5.23	118.44	111.75
1	C	441	GLY	N-CA-C	-5.22	101.69	112.34
1	F	337	ASP	N-CA-C	-5.19	105.31	111.69
1	B	103	VAL	CA-C-N	-5.16	116.41	122.14
1	B	103	VAL	C-N-CA	-5.16	116.41	122.14
1	D	549	PRO	CA-C-N	-5.12	114.44	119.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	549	PRO	C-N-CA	-5.12	114.44	119.92
1	B	584	GLY	N-CA-C	-5.09	106.59	112.29
1	B	483	SER	CA-C-N	-5.07	114.56	120.04
1	B	483	SER	C-N-CA	-5.07	114.56	120.04
1	F	515	TYR	N-CA-C	-5.05	102.90	110.23
1	B	437	ASP	N-CA-CB	-5.02	101.78	110.32
1	B	333	SER	N-CA-C	5.01	116.82	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	333	SER	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5236	0	5107	74	0
1	B	5238	0	5106	78	0
1	C	5236	0	5092	76	0
1	D	5232	0	5096	50	0
1	E	5268	0	5154	71	0
1	F	5233	0	5103	60	0
2	A	30	0	40	9	0
2	B	42	0	56	16	0
2	C	36	0	48	7	0
2	D	24	0	32	4	0
2	E	24	0	32	11	0
2	F	30	0	40	7	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	A	2	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	1	0
4	E	2	0	0	1	0
4	F	2	0	0	0	0
5	A	3	0	7	5	0
5	B	3	0	7	2	0
5	C	3	0	7	1	0
5	D	3	0	7	0	0
5	E	3	0	7	0	0
5	F	3	0	7	2	0
6	C	5	0	0	1	0
7	A	571	0	0	17	0
7	B	656	0	0	11	0
7	C	537	0	0	16	0
7	D	498	0	0	7	0
7	E	519	0	0	12	0
7	F	559	0	0	13	0
All	All	35006	0	30948	404	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 6.

All (404) 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:E:624:HIS:HE1	1:E:634[C]:MET:HE1	1.20	1.07
1:D:23:HIS:HE2	2:D:702:GOL:H11	1.21	1.02
1:E:642:MET:HE3	1:E:644[B]:ARG:NH1	1.74	1.01
1:C:328[B]:MET:HE2	7:C:1217:HOH:O	1.62	0.98
1:F:437:ASP:HB2	7:F:986:HOH:O	1.65	0.97
1:C:644:ARG:HD2	7:C:1271:HOH:O	1.64	0.96
1:D:68:LYS:HE3	2:D:702:GOL:H2	1.43	0.95
1:A:352:ARG:HD3	7:A:1266:HOH:O	1.65	0.94
1:E:23:HIS:HD2	1:E:25:LEU:H	1.16	0.91
1:B:558[B]:LEU:HD23	2:B:701:GOL:H2	1.54	0.90
1:A:332:LEU:O	1:A:333:SER:HB3	1.73	0.89
1:B:414:MET:HE3	1:B:418:ALA:HB3	1.55	0.88
1:F:336:CYS:HB3	7:F:1207:HOH:O	1.73	0.88
1:C:214:LYS:O	2:C:704:GOL:H12	1.74	0.87
1:A:168:LYS:HB2	1:A:170[B]:LEU:HD11	1.55	0.87
1:A:68:LYS:HE3	2:A:703:GOL:H31	1.57	0.87
1:C:116:LEU:CD1	1:C:157[A]:THR:HG23	2.05	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:624:HIS:CE1	1:E:634[C]:MET:HE1	2.09	0.86
1:C:23:HIS:HD2	1:C:25:LEU:H	1.23	0.86
1:E:634[A]:MET:HE1	4:E:706:PEO:O2	1.77	0.85
1:A:336:CYS:HB3	7:A:1254:HOH:O	1.76	0.84
1:C:116:LEU:HD12	1:C:157[A]:THR:HG23	1.60	0.84
1:A:352:ARG:CD	7:A:1266:HOH:O	2.23	0.84
1:B:74:LEU:HD13	1:B:74:LEU:C	2.02	0.84
1:E:68:LYS:HE3	2:E:704:GOL:H11	1.59	0.84
1:A:23:HIS:HD2	1:A:25:LEU:H	1.23	0.83
1:E:642:MET:HE3	1:E:644[B]:ARG:HH11	1.41	0.82
1:E:506:LYS:HE3	7:E:1248:HOH:O	1.79	0.80
1:F:360:LYS:HE2	7:F:1324:HOH:O	1.82	0.80
1:B:558[B]:LEU:HD21	2:B:701:GOL:H31	1.62	0.80
1:B:437:ASP:HB2	7:B:965:HOH:O	1.82	0.80
2:F:704:GOL:H11	7:F:1256:HOH:O	1.82	0.80
1:B:558[B]:LEU:CD2	2:B:701:GOL:H2	2.12	0.79
1:D:122[B]:CYS:HB2	7:D:1282:HOH:O	1.83	0.78
1:A:405:TYQ:HN51	5:A:708:NEH:HA2	1.49	0.78
1:D:280:ASP:OD2	2:D:702:GOL:H12	1.86	0.76
1:B:218:HIS:ND1	2:B:707:GOL:H12	2.03	0.74
1:E:265:LYS:HE2	2:E:704:GOL:H12	1.71	0.73
1:D:122[A]:CYS:HB3	7:D:1282:HOH:O	1.89	0.73
1:A:670:ARG:NH1	7:A:1294:HOH:O	2.23	0.71
1:C:23:HIS:HE1	2:C:702:GOL:O3	1.75	0.70
1:E:527:ASN:C	1:E:527:ASN:HD22	2.00	0.70
1:F:68:LYS:HE3	2:F:702:GOL:O2	1.92	0.69
1:B:527:ASN:C	1:B:527:ASN:HD22	2.00	0.69
1:F:338:CYS:HB3	1:F:364[B]:CYS:SG	2.32	0.69
1:F:642:MET:HE1	1:F:644[B]:ARG:HH21	1.58	0.69
1:E:333:SER:HB2	7:E:1120:HOH:O	1.93	0.69
4:A:707:PEO:O1	7:A:1365:HOH:O	2.10	0.68
2:C:703:GOL:H31	7:C:1142:HOH:O	1.90	0.68
1:A:669:LYS:HD3	7:B:1200:HOH:O	1.93	0.68
1:C:333:SER:HB2	1:C:344:TYR:OH	1.93	0.68
1:B:558[B]:LEU:CD2	2:B:701:GOL:C2	2.71	0.67
1:A:333:SER:HB2	1:A:344:TYR:OH	1.93	0.67
1:B:265:LYS:HD3	2:B:704:GOL:H2	1.77	0.67
1:F:527:ASN:HD22	1:F:529:ASN:H	1.43	0.67
1:F:333:SER:HB3	1:F:361:ASN:OD1	1.95	0.67
1:A:122[B]:CYS:SG	7:A:1338:HOH:O	2.52	0.67
1:B:218:HIS:HB3	2:B:707:GOL:C1	2.25	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:SER:CB	1:C:344:TYR:OH	2.44	0.66
1:E:333:SER:CB	7:E:1120:HOH:O	2.42	0.66
1:C:366:HIS:HE1	7:C:1100:HOH:O	1.78	0.66
1:C:527:ASN:HD22	1:C:529:ASN:H	1.44	0.65
1:C:260:GLU:HG2	1:C:265:LYS:HG3	1.77	0.65
1:F:168:LYS:HE2	7:F:1046:HOH:O	1.97	0.65
1:B:558[B]:LEU:HD21	2:B:701:GOL:C3	2.27	0.65
1:B:348:HIS:HD2	7:B:1196:HOH:O	1.80	0.65
1:C:427:GLY:O	1:C:634[A]:MET:HG2	1.97	0.65
1:A:527:ASN:C	1:A:527:ASN:HD22	2.06	0.64
1:A:116:LEU:CD1	1:A:157[A]:THR:HG23	2.28	0.63
1:A:122[A]:CYS:SG	7:A:1351:HOH:O	2.55	0.63
1:B:567:SER:HB3	7:B:1406:HOH:O	1.97	0.63
1:A:23:HIS:HE1	2:A:703:GOL:C1	2.11	0.63
1:F:501:GLU:OE2	7:F:929:HOH:O	2.16	0.63
1:F:527:ASN:HD21	1:F:529:ASN:HD22	1.44	0.63
1:A:556:GLY:O	7:A:1159:HOH:O	2.15	0.63
2:E:703:GOL:H31	7:E:1272:HOH:O	1.97	0.63
1:D:48:LYS:HG2	7:D:1044:HOH:O	1.98	0.62
1:E:106:THR:OG1	7:E:1177:HOH:O	2.15	0.62
1:B:644:ARG:HD2	7:B:1449:HOH:O	2.00	0.62
1:B:313:GLN:H	1:B:313:GLN:HE21	1.47	0.62
1:A:146:ASN:H	1:A:146:ASN:HD22	1.47	0.62
1:F:265:LYS:HE3	2:F:702:GOL:H2	1.81	0.61
1:B:558[B]:LEU:HD23	2:B:701:GOL:C2	2.27	0.61
1:D:414:MET:CE	1:D:420:ARG:HB2	2.31	0.61
1:D:527:ASN:HD22	1:D:529:ASN:H	1.46	0.61
1:A:405:TYQ:HN51	5:A:708:NEH:CA	2.13	0.61
1:C:116:LEU:HD11	1:C:157[A]:THR:HG23	1.82	0.61
1:F:34:LYS:NZ	7:F:1272:HOH:O	2.32	0.61
1:A:405:TYQ:N5	5:A:708:NEH:HA2	2.15	0.61
1:E:631:PHE:CG	1:E:632:PRO:HA	2.37	0.60
1:F:148:MET:HE2	1:F:148:MET:HA	1.83	0.60
1:F:338:CYS:SG	1:F:364[B]:CYS:CB	2.88	0.60
1:C:313:GLN:H	1:C:313:GLN:HE21	1.50	0.60
1:C:527:ASN:HD22	1:C:527:ASN:C	2.10	0.60
1:F:217:LYS:HE2	1:F:217:LYS:HA	1.84	0.60
1:C:631:PHE:CG	1:C:632:PRO:HA	2.37	0.59
1:F:444:GLY:HA3	1:F:452:ASN:HD21	1.66	0.59
1:B:338:CYS:HB3	1:B:364[B]:CYS:SG	2.41	0.59
1:B:558[B]:LEU:HD21	2:B:701:GOL:C2	2.31	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:567[B]:SER:OG	7:C:1252:HOH:O	2.16	0.59
1:D:575:TYR:O	1:D:576:LYS:HD2	2.01	0.59
1:E:23:HIS:CD2	1:E:25:LEU:H	2.08	0.59
1:B:74:LEU:C	1:B:74:LEU:CD1	2.74	0.59
1:B:218:HIS:HB3	2:B:707:GOL:H12	1.84	0.59
1:C:121:LEU:HD12	1:C:328[B]:MET:HE1	1.84	0.59
1:F:21:PRO:HG3	1:F:77:ARG:CZ	2.32	0.59
1:E:425:LEU:HB3	7:E:1144:HOH:O	2.01	0.59
1:A:157[A]:THR:HG21	1:A:588:PRO:HB3	1.84	0.59
1:E:442:PRO:HG3	2:F:706:GOL:H31	1.84	0.59
1:E:671:ALA:O	1:E:672:VAL:HG12	2.03	0.59
1:F:642:MET:CE	1:F:644[B]:ARG:HH21	2.14	0.58
1:E:444:GLY:HA3	1:E:452:ASN:HD21	1.69	0.58
1:E:527:ASN:HD22	1:E:529:ASN:H	1.50	0.58
1:B:634[B]:MET:HE1	4:B:708:PEO:O1	2.03	0.58
1:F:642:MET:CE	1:F:644[B]:ARG:HE	2.17	0.58
1:F:366:HIS:HE1	1:F:368:GLU:OE2	1.87	0.58
1:F:313:GLN:H	1:F:313:GLN:HE21	1.51	0.58
1:B:74:LEU:HD13	1:B:75:PRO:N	2.18	0.57
1:E:427:GLY:O	1:E:634[C]:MET:HG2	2.04	0.57
1:A:644:ARG:HD2	7:A:1256:HOH:O	2.04	0.57
1:B:260:GLU:HG2	1:B:265:LYS:HG3	1.85	0.57
1:E:333:SER:HA	1:E:335:GLY:N	2.19	0.57
1:B:527:ASN:HD22	1:B:529:ASN:H	1.53	0.57
1:E:157:THR:HG22	7:E:1054:HOH:O	2.04	0.57
1:C:20:ARG:HD2	1:C:74:LEU:HD21	1.86	0.57
1:F:405:TYQ:N5	5:F:708:NEH:N	2.53	0.57
1:A:527:ASN:HD22	1:A:529:ASN:H	1.53	0.56
1:B:218:HIS:HB3	2:B:707:GOL:H11	1.86	0.56
1:B:20:ARG:NH1	1:B:74:LEU:HD11	2.19	0.56
1:F:527:ASN:HD22	1:F:527:ASN:C	2.14	0.56
1:B:338:CYS:SG	1:B:364[B]:CYS:CB	2.94	0.56
1:D:631:PHE:CG	1:D:632:PRO:HA	2.41	0.56
1:D:642:MET:HE3	1:D:644[B]:ARG:CZ	2.36	0.56
1:F:527:ASN:ND2	1:F:529:ASN:HD22	2.04	0.56
1:A:23:HIS:CD2	1:A:25:LEU:H	2.14	0.56
1:B:68:LYS:HE3	2:B:704:GOL:H11	1.86	0.56
1:D:527:ASN:HD22	1:D:527:ASN:C	2.14	0.56
1:E:481[B]:LYS:NZ	7:E:996:HOH:O	2.38	0.55
1:B:21:PRO:HG3	1:B:77:ARG:CZ	2.36	0.55
1:D:301:MET:HE3	1:D:460:PHE:CE2	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506[A]:LYS:HG3	7:A:1208:HOH:O	2.05	0.55
1:A:631:PHE:CG	1:A:632:PRO:HA	2.42	0.55
1:B:414:MET:HE3	1:B:418:ALA:CB	2.33	0.55
1:A:219:LYS:H	2:A:704:GOL:H32	1.72	0.55
1:C:181:GLU:HG2	7:C:801:HOH:O	2.07	0.55
1:B:119:GLU:HB3	1:B:352:ARG:NH1	2.21	0.54
1:E:631:PHE:CD1	1:E:632:PRO:HA	2.42	0.54
1:B:425:LEU:HB3	7:B:1309:HOH:O	2.07	0.54
1:B:670:ARG:NH2	7:B:921:HOH:O	2.40	0.54
1:E:414:MET:HE3	1:E:418:ALA:HB3	1.90	0.54
1:D:70:GLN:HG2	7:D:1210:HOH:O	2.07	0.54
1:D:414:MET:HE2	1:D:420:ARG:HB2	1.89	0.54
1:C:402:ALA:O	1:C:405:TYQ:HD2	2.07	0.54
1:A:157[A]:THR:HB	1:A:159:GLY:H	1.72	0.53
1:E:672:VAL:HA	7:E:1196:HOH:O	2.08	0.53
1:F:214:LYS:O	2:F:705:GOL:O3	2.24	0.53
1:B:313:GLN:H	1:B:313:GLN:NE2	2.06	0.53
1:C:116:LEU:HD11	1:C:157[A]:THR:CG2	2.38	0.53
1:D:444:GLY:HA3	1:D:452:ASN:HD21	1.72	0.53
1:C:313:GLN:H	1:C:313:GLN:NE2	2.06	0.53
1:E:265:LYS:CE	2:E:704:GOL:H12	2.39	0.53
1:C:414:MET:HE3	1:C:418:ALA:HB3	1.90	0.53
1:A:497:ALA:HB2	1:B:308:PRO:HB3	1.90	0.53
1:A:305:TYR:CD2	1:A:456:HIS:HB3	2.44	0.53
1:E:527:ASN:ND2	1:E:529:ASN:H	2.07	0.53
1:C:313:GLN:HG3	1:D:494:TYR:CD1	2.44	0.52
1:F:210:ASN:HB3	7:F:1300:HOH:O	2.09	0.52
1:E:344:TYR:HB3	1:E:361:ASN:HD22	1.73	0.52
1:A:631:PHE:CD1	1:A:632:PRO:HA	2.44	0.52
1:D:338:CYS:HB3	1:D:364[B]:CYS:SG	2.50	0.52
1:C:390:ARG:HG3	1:C:660:SER:OG	2.10	0.52
1:F:313:GLN:H	1:F:313:GLN:NE2	2.07	0.52
1:A:390:ARG:HG3	1:A:660:SER:OG	2.10	0.52
1:B:50:SER:HB2	1:B:352:ARG:HG3	1.91	0.52
1:B:427:GLY:O	1:B:634[A]:MET:HG2	2.09	0.52
1:C:160:TYR:CD2	1:C:558:LEU:HD21	2.45	0.52
1:D:343:HIS:HB2	2:D:705:GOL:H2	1.90	0.52
1:E:645:PRO:O	1:E:646:ARG:HD2	2.10	0.52
1:C:21:PRO:HG3	1:C:77:ARG:CZ	2.40	0.52
1:A:68:LYS:HE3	2:A:703:GOL:C3	2.35	0.51
1:A:527:ASN:HD21	1:A:529:ASN:HB2	1.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:338:CYS:CB	1:F:364[B]:CYS:SG	2.97	0.51
1:F:527:ASN:ND2	1:F:529:ASN:H	2.06	0.51
1:C:344:TYR:CB	1:C:361:ASN:HD22	2.23	0.51
1:C:631:PHE:CD1	1:C:632:PRO:HA	2.46	0.51
1:E:375:LYS:HE2	7:F:1024:HOH:O	2.09	0.51
1:F:631:PHE:CG	1:F:632:PRO:HA	2.45	0.51
1:A:116:LEU:HD12	1:A:157[A]:THR:HG23	1.93	0.51
1:D:338:CYS:SG	1:D:364[B]:CYS:SG	3.08	0.51
1:E:54[B]:VAL:HG22	1:E:350:SER:HB2	1.92	0.51
1:B:334:LEU:HD12	7:B:1426:HOH:O	2.10	0.51
1:C:452:ASN:C	1:C:452:ASN:HD22	2.18	0.51
1:E:580:LEU:HD21	2:E:705:GOL:H11	1.93	0.51
1:C:296:ILE:HD12	1:C:464:ILE:HG12	1.92	0.51
1:C:444:GLY:HA3	1:C:452:ASN:HD21	1.75	0.51
1:B:444:GLY:HA3	1:B:452:ASN:HD21	1.76	0.50
1:A:23:HIS:CE1	2:A:703:GOL:C1	2.93	0.50
1:D:74:LEU:HB2	7:D:890:HOH:O	2.10	0.50
1:F:222:ASN:HB3	1:F:227:HIS:CG	2.46	0.50
1:C:527:ASN:HD21	1:C:529:ASN:HD22	1.57	0.50
1:C:527:ASN:ND2	1:C:529:ASN:H	2.09	0.50
1:E:68:LYS:CE	2:E:704:GOL:H11	2.37	0.50
1:E:332:LEU:O	1:E:333:SER:C	2.54	0.50
1:D:527:ASN:HD21	1:D:529:ASN:HD22	1.59	0.50
1:E:644[B]:ARG:HD2	7:E:1018:HOH:O	2.13	0.49
1:A:332:LEU:O	1:A:333:SER:CB	2.48	0.49
1:C:23:HIS:CE1	2:C:702:GOL:O3	2.61	0.49
1:C:146:ASN:C	1:C:146:ASN:HD22	2.20	0.49
1:E:644[A]:ARG:NH1	7:E:1251:HOH:O	2.45	0.49
1:C:527:ASN:ND2	1:C:529:ASN:HD22	2.11	0.49
1:A:219:LYS:HB3	7:A:1344:HOH:O	2.11	0.49
1:A:313:GLN:H	1:A:313:GLN:HE21	1.61	0.49
1:E:211[A]:ARG:HG3	1:E:213:ARG:HD2	1.95	0.49
1:A:352:ARG:HD2	7:A:1266:HOH:O	2.02	0.49
1:C:116:LEU:CD1	1:C:157[A]:THR:CG2	2.86	0.49
1:E:344:TYR:CB	1:E:361:ASN:HD22	2.26	0.49
1:E:527:ASN:HD21	1:E:529:ASN:HD22	1.59	0.49
1:E:21:PRO:HG3	1:E:77:ARG:CZ	2.42	0.49
1:E:452:ASN:HD22	1:E:453:ALA:N	2.11	0.49
2:A:706:GOL:H31	7:A:1310:HOH:O	2.13	0.48
1:B:218:HIS:CB	2:B:707:GOL:H12	2.42	0.48
1:B:218:HIS:HD2	1:B:450:ASN:HD22	1.60	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:634[A]:MET:HE1	7:B:1310:HOH:O	2.12	0.48
1:E:452:ASN:HD22	1:E:452:ASN:C	2.21	0.48
1:B:330:ASN:O	1:B:332:LEU:HD13	2.13	0.48
1:B:402:ALA:O	1:B:405:TYQ:HD2	2.14	0.48
1:E:68:LYS:HE3	2:E:704:GOL:C1	2.37	0.48
1:A:258:VAL:HG22	2:A:703:GOL:H11	1.95	0.48
1:A:374:PHE:CD1	1:B:633:LEU:HD13	2.48	0.48
1:C:145:ALA:O	1:C:148:MET:HG2	2.13	0.48
1:A:23:HIS:HE1	2:A:703:GOL:H12	1.79	0.48
1:A:116:LEU:HD11	1:A:157[A]:THR:HG23	1.94	0.48
1:A:168:LYS:O	1:A:170[B]:LEU:CD1	2.62	0.48
1:C:328[B]:MET:HB3	1:C:401:THR:O	2.14	0.48
1:C:344:TYR:HB3	1:C:361:ASN:HD22	1.78	0.48
1:C:637:GLU:HG2	7:C:832[B]:HOH:O	2.13	0.48
1:C:333:SER:HB3	1:C:344:TYR:OH	2.13	0.48
1:D:481[A]:LYS:NZ	7:D:1160:HOH:O	2.33	0.48
1:A:366:HIS:CE1	7:A:1181:HOH:O	2.66	0.47
1:B:222:ASN:HB3	1:B:227:HIS:CG	2.49	0.47
1:C:527:ASN:HD21	1:C:529:ASN:HB2	1.79	0.47
1:A:444:GLY:HA3	1:A:452:ASN:HD21	1.79	0.47
1:D:301:MET:O	1:D:318:LEU:HA	2.13	0.47
1:C:62:LYS:O	1:C:66:GLN:HG3	2.14	0.47
1:A:169:ARG:C	1:A:170[B]:LEU:HD12	2.39	0.47
1:A:402:ALA:O	1:A:405:TYQ:HD2	2.14	0.47
1:A:333:SER:HB2	1:A:344:TYR:CZ	2.49	0.47
1:B:265:LYS:HD3	2:B:704:GOL:C2	2.43	0.47
1:B:338:CYS:CB	1:B:364[B]:CYS:SG	3.02	0.47
1:C:121:LEU:HD12	1:C:328[B]:MET:CE	2.44	0.47
1:D:414:MET:HE1	1:D:420:ARG:HB2	1.95	0.47
1:B:426:THR:HA	1:B:634[A]:MET:HG3	1.97	0.47
1:B:567:SER:CB	7:B:1406:HOH:O	2.61	0.47
1:E:160:TYR:CD2	1:E:558:LEU:HD21	2.50	0.47
1:D:186:TYR:CD2	1:D:428:ILE:HG21	2.50	0.47
1:E:527:ASN:C	1:E:527:ASN:ND2	2.72	0.47
1:B:17:ALA:C	7:B:1144:HOH:O	2.57	0.46
1:B:375:LYS:HG3	1:B:388:VAL:HG22	1.96	0.46
1:E:374:PHE:CD1	1:F:633:LEU:HD13	2.49	0.46
1:A:509:LYS:HE2	7:A:999:HOH:O	2.14	0.46
1:C:157[B]:THR:HG23	1:C:159:GLY:N	2.29	0.46
1:D:217:LYS:HE3	7:D:1083:HOH:O	2.15	0.46
2:C:704:GOL:H32	7:C:979:HOH:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:527:ASN:ND2	1:D:529:ASN:H	2.11	0.46
1:F:265:LYS:HE3	2:F:702:GOL:C2	2.44	0.46
1:F:360:LYS:CE	7:F:1324:HOH:O	2.53	0.46
1:B:20:ARG:HB2	1:B:21:PRO:HD2	1.98	0.46
1:A:222:ASN:HB3	1:A:227:HIS:CG	2.50	0.46
1:A:333:SER:O	1:A:335:GLY:O	2.34	0.46
1:F:259:MET:CE	1:F:365:ILE:HG21	2.46	0.46
1:B:20:ARG:CZ	1:B:74:LEU:HD11	2.45	0.46
1:D:338:CYS:SG	1:D:364[B]:CYS:CB	3.04	0.46
1:F:338:CYS:CB	1:F:364[B]:CYS:HG	2.28	0.46
1:B:156:TRP:CE2	5:B:709:NEH:HA2	2.51	0.46
1:C:23:HIS:CD2	1:C:25:LEU:H	2.15	0.46
1:C:157[B]:THR:HG23	1:C:159:GLY:H	1.80	0.46
1:C:222:ASN:HB3	1:C:227:HIS:CG	2.50	0.46
1:D:402:ALA:O	1:D:405:TYQ:HD2	2.16	0.46
1:F:71:GLY:HA2	7:F:1160:HOH:O	2.16	0.46
1:F:375:LYS:HG3	1:F:388:VAL:HG22	1.98	0.46
1:C:578[B]:ASN:ND2	7:C:1255:HOH:O	2.49	0.45
1:B:119:GLU:HB3	1:B:352:ARG:HH12	1.81	0.45
1:C:313:GLN:HG3	1:D:494:TYR:CG	2.51	0.45
1:F:20:ARG:HE	1:F:20:ARG:HB3	1.55	0.45
1:F:360:LYS:HB3	1:F:360:LYS:HE3	1.54	0.45
1:A:168:LYS:HB2	1:A:170[B]:LEU:CD1	2.38	0.45
1:A:313:GLN:H	1:A:313:GLN:NE2	2.14	0.45
1:C:405:TYQ:N5	5:C:708:NEH:N	2.63	0.45
1:C:669:LYS:HE3	1:D:181:GLU:OE1	2.16	0.45
1:A:168:LYS:C	1:A:170[B]:LEU:HD12	2.41	0.45
1:B:218:HIS:CG	2:B:707:GOL:H12	2.51	0.45
1:B:342:ILE:HG23	1:B:364[B]:CYS:SG	2.56	0.45
1:E:578[A]:ASN:H	2:E:705:GOL:H12	1.82	0.45
1:B:217:LYS:HA	1:B:217:LYS:HD2	1.88	0.45
1:B:631:PHE:CG	1:B:632:PRO:HA	2.52	0.45
1:C:339:LYS:HE3	7:C:1187:HOH:O	2.17	0.45
1:F:631:PHE:CD1	1:F:632:PRO:HA	2.51	0.45
1:C:199:GLU:HG3	7:C:1174:HOH:O	2.17	0.45
1:E:578[B]:ASN:H	2:E:705:GOL:H12	1.82	0.45
1:C:485:TYR:O	1:D:554:LYS:HE3	2.16	0.45
1:E:414:MET:HE2	1:E:420:ARG:HB2	1.97	0.45
1:C:332:LEU:O	1:C:333:SER:CB	2.64	0.45
1:D:94:GLY:HA3	1:D:105:GLU:O	2.16	0.45
1:E:199[B]:GLU:HG3	1:E:200:GLU:N	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:644[A]:ARG:NH2	7:F:1213:HOH:O	2.44	0.45
1:A:427:GLY:O	1:A:634[A]:MET:HG2	2.17	0.44
1:A:157[A]:THR:CG2	1:A:588:PRO:HB3	2.48	0.44
1:C:509:LYS:NZ	7:C:1156:HOH:O	2.49	0.44
1:E:642:MET:CE	1:E:644[B]:ARG:NH1	2.63	0.44
1:C:434:LEU:HB2	1:C:452:ASN:HB2	2.00	0.44
1:D:222:ASN:HB3	1:D:227:HIS:CG	2.52	0.44
1:C:587:VAL:O	1:C:588:PRO:C	2.61	0.44
1:F:323:TYR:CE2	5:F:708:NEH:HA3	2.53	0.44
1:F:222:ASN:O	1:F:231:LYS:NZ	2.50	0.44
1:E:305:TYR:OH	1:E:405:TYQ:OH	2.31	0.44
1:C:369[B]:ASP:OD2	1:D:339:LYS:HD2	2.18	0.43
1:C:497:ALA:HB2	1:D:308:PRO:HB3	1.99	0.43
1:D:342:ILE:HG21	1:D:344:TYR:CZ	2.54	0.43
1:E:213:ARG:HH21	1:E:438:GLU:CD	2.26	0.43
1:B:254:MET:HE3	1:B:259:MET:HB2	1.99	0.43
1:B:135:ILE:HG12	1:B:148:MET:HG3	2.00	0.43
1:B:303:VAL:HA	1:B:457:GLN:O	2.19	0.43
1:E:642:MET:CE	1:E:644[B]:ARG:HH11	2.22	0.43
1:A:241:PRO:HD2	1:B:248:GLU:HB2	1.99	0.43
1:E:655:LEU:HD22	1:F:223:PHE:HB2	2.00	0.43
1:B:468:ILE:O	1:B:527:ASN:HB2	2.18	0.43
1:C:519:THR:O	1:C:520:GLY:C	2.60	0.43
1:D:37:THR:HG22	1:D:51:PHE:CE2	2.53	0.43
1:F:414:MET:HE3	1:F:418:ALA:HB3	2.01	0.43
1:A:452:ASN:C	1:A:452:ASN:HD22	2.26	0.43
1:A:527:ASN:ND2	1:A:529:ASN:H	2.14	0.43
1:B:575:TYR:CD2	1:B:575:TYR:C	2.96	0.43
1:E:74:LEU:HA	1:E:75:PRO:HD3	1.84	0.43
1:D:631:PHE:CD1	1:D:632:PRO:HA	2.53	0.43
2:E:705:GOL:H32	7:E:1020:HOH:O	2.18	0.43
1:B:222:ASN:HB3	1:B:227:HIS:ND1	2.34	0.43
1:B:527:ASN:C	1:B:527:ASN:ND2	2.74	0.43
1:C:116:LEU:HD13	1:C:121:LEU:HD21	2.01	0.43
2:E:703:GOL:H12	1:F:442:PRO:HG3	2.01	0.43
1:F:652:ASN:OD1	1:F:652:ASN:C	2.61	0.43
1:F:472:GLY:C	1:F:473:ASN:HD22	2.26	0.43
1:D:20:ARG:HE	1:D:20:ARG:HB3	1.27	0.43
1:A:188:HIS:CD2	1:A:216:SER:HB3	2.53	0.42
2:C:705:GOL:H2	7:C:857:HOH:O	2.18	0.42
1:E:175[B]:VAL:HG23	1:E:190:LEU:HB2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:48:LYS:HD2	1:F:48:LYS:HA	1.80	0.42
1:C:425:LEU:HD23	7:C:1225:HOH:O	2.19	0.42
1:D:313:GLN:H	1:D:313:GLN:HE21	1.68	0.42
1:E:333:SER:HA	1:E:334:LEU:C	2.44	0.42
1:B:575:TYR:O	1:B:576[B]:LYS:HD3	2.19	0.42
1:C:303:VAL:HA	1:C:457:GLN:O	2.19	0.42
1:E:144:PRO:HB2	1:E:146:ASN:ND2	2.34	0.42
1:E:222:ASN:HB3	1:E:227:HIS:CG	2.54	0.42
1:F:265:LYS:HG2	2:F:702:GOL:H2	2.01	0.42
1:F:575:TYR:CD1	1:F:575:TYR:C	2.97	0.42
1:D:135:ILE:HG12	1:D:148:MET:HG3	2.02	0.42
1:D:338:CYS:CB	1:D:364[B]:CYS:SG	3.08	0.42
1:F:168:LYS:CE	7:F:1046:HOH:O	2.61	0.42
1:F:642:MET:HE3	1:F:644[B]:ARG:HE	1.83	0.42
1:A:160:TYR:CD2	1:A:558:LEU:HD21	2.54	0.42
1:A:217:LYS:HA	1:A:217:LYS:HD2	1.63	0.42
1:A:361:ASN:ND2	7:A:966:HOH:O	2.52	0.42
1:A:628:PRO:O	1:B:651:GLU:HA	2.20	0.42
1:B:631:PHE:CD1	1:B:632:PRO:HA	2.55	0.42
1:F:366:HIS:CE1	1:F:368:GLU:OE2	2.70	0.42
1:C:215:VAL:O	2:C:704:GOL:H31	2.20	0.42
1:E:425:LEU:HD12	1:E:622:ILE:HD11	2.02	0.42
1:F:642:MET:HE3	1:F:644[B]:ARG:NE	2.34	0.42
1:C:452:ASN:HD22	1:C:453:ALA:N	2.17	0.42
1:E:402:ALA:O	1:E:405:TYQ:HD2	2.20	0.42
1:F:414:MET:SD	1:F:420:ARG:NH1	2.93	0.42
1:B:527:ASN:HD21	1:B:529:ASN:HD22	1.68	0.41
1:C:219:LYS:HG3	6:C:709:PO4:O3	2.19	0.41
1:C:333:SER:HB3	1:C:344:TYR:CZ	2.55	0.41
1:E:644[B]:ARG:HG2	1:E:646:ARG:HD3	2.03	0.41
1:A:405:TYQ:N5	5:A:708:NEH:CA	2.81	0.41
1:A:405:TYQ:N5	5:A:708:NEH:N	2.67	0.41
1:D:364[B]:CYS:SG	1:D:366:HIS:CD2	3.14	0.41
1:E:217:LYS:HA	1:E:217:LYS:HD2	1.96	0.41
1:E:176:TYR:CE1	1:E:189:PRO:HB3	2.55	0.41
1:C:405:TYQ:CD2	7:C:1223:HOH:O	2.68	0.41
1:F:26:ASP:O	1:F:56:LEU:HD22	2.20	0.41
1:D:311:PRO:HA	1:D:313:GLN:HE22	1.85	0.41
1:D:498:PHE:CD1	1:D:498:PHE:C	2.99	0.41
1:E:458:HIS:O	1:E:621:GLY:HA3	2.20	0.41
1:A:429:LEU:HD11	1:A:630:ASP:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:261:TRP:O	1:E:262:SER:C	2.64	0.41
1:E:414:MET:HE3	1:E:418:ALA:CB	2.50	0.41
1:A:303:VAL:HA	1:A:457:GLN:O	2.21	0.41
1:A:125:GLU:HG3	7:A:976:HOH:O	2.21	0.41
1:A:144:PRO:HB2	1:A:146:ASN:ND2	2.36	0.41
1:B:405:TYQ:N5	5:B:709:NEH:N	2.69	0.41
1:C:578[B]:ASN:CG	7:C:1255:HOH:O	2.64	0.41
1:A:68:LYS:CE	2:A:703:GOL:H31	2.38	0.41
1:B:527:ASN:ND2	1:B:529:ASN:H	2.15	0.41
1:C:374:PHE:CD1	1:D:633:LEU:HD13	2.56	0.41
1:B:53:THR:O	1:B:81:TYR:HA	2.21	0.40
1:B:634[A]:MET:HA	1:B:635:PRO:HD3	1.97	0.40
1:F:262:SER:O	1:F:263:ASN:HB2	2.20	0.40
1:B:634[A]:MET:HE3	1:B:634[A]:MET:HB2	1.76	0.40
1:D:359:VAL:HG22	1:D:362:ALA:HB2	2.03	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	664/692 (96%)	636 (96%)	27 (4%)	1 (0%)	43	49
1	B	663/692 (96%)	637 (96%)	25 (4%)	1 (0%)	43	49
1	C	665/692 (96%)	639 (96%)	23 (4%)	3 (0%)	24	25
1	D	661/692 (96%)	632 (96%)	29 (4%)	0	100	100
1	E	669/692 (97%)	640 (96%)	27 (4%)	2 (0%)	36	39
1	F	661/692 (96%)	633 (96%)	25 (4%)	3 (0%)	24	25
All	All	3983/4152 (96%)	3817 (96%)	156 (4%)	10 (0%)	43	39

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	19	ALA
1	E	333	SER
1	F	22	ALA
1	F	335	GLY
1	C	403	ALA
1	A	333	SER
1	C	336[A]	CYS
1	C	336[B]	CYS
1	E	403	ALA
1	B	403	ALA

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	576/593 (97%)	552 (96%)	24 (4%)	26	32
1	B	575/593 (97%)	552 (96%)	23 (4%)	28	35
1	C	576/593 (97%)	554 (96%)	22 (4%)	29	37
1	D	574/593 (97%)	549 (96%)	25 (4%)	25	31
1	E	582/593 (98%)	564 (97%)	18 (3%)	35	45
1	F	574/593 (97%)	554 (96%)	20 (4%)	32	40
All	All	3457/3558 (97%)	3325 (96%)	132 (4%)	31	37

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LYS
1	A	84	LEU
1	A	122[A]	CYS
1	A	122[B]	CYS
1	A	126[A]	GLU
1	A	126[B]	GLU
1	A	146	ASN
1	A	157[A]	THR
1	A	157[B]	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	201	LYS
1	A	213	ARG
1	A	217	LYS
1	A	238	GLU
1	A	313	GLN
1	A	329	THR
1	A	334	LEU
1	A	360	LYS
1	A	364	CYS
1	A	382	ASN
1	A	394	LEU
1	A	481[A]	LYS
1	A	481[B]	LYS
1	A	527	ASN
1	A	531	VAL
1	B	20	ARG
1	B	74	LEU
1	B	84	LEU
1	B	109	LEU
1	B	122	CYS
1	B	201	LYS
1	B	202	LYS
1	B	217	LYS
1	B	238	GLU
1	B	244	VAL
1	B	265	LYS
1	B	313	GLN
1	B	329	THR
1	B	332	LEU
1	B	334	LEU
1	B	359	VAL
1	B	369	ASP
1	B	421	LEU
1	B	437	ASP
1	B	527	ASN
1	B	576[A]	LYS
1	B	576[B]	LYS
1	B	633	LEU
1	C	20	ARG
1	C	102[A]	SER
1	C	102[B]	SER
1	C	146	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	157[A]	THR
1	C	157[B]	THR
1	C	202	LYS
1	C	213	ARG
1	C	255	THR
1	C	313	GLN
1	C	329	THR
1	C	334	LEU
1	C	336[A]	CYS
1	C	336[B]	CYS
1	C	360	LYS
1	C	364	CYS
1	C	382	ASN
1	C	394	LEU
1	C	527	ASN
1	C	531	VAL
1	C	641	LEU
1	C	670	ARG
1	D	20	ARG
1	D	42	SER
1	D	48	LYS
1	D	84	LEU
1	D	109	LEU
1	D	143	ILE
1	D	202	LYS
1	D	211	ARG
1	D	217	LYS
1	D	248	GLU
1	D	254	MET
1	D	313	GLN
1	D	329	THR
1	D	334	LEU
1	D	338	CYS
1	D	352	ARG
1	D	357	ILE
1	D	359	VAL
1	D	360	LYS
1	D	369	ASP
1	D	421	LEU
1	D	527	ASN
1	D	576	LYS
1	D	633	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	660	SER
1	E	20	ARG
1	E	84	LEU
1	E	88	LYS
1	E	101	LEU
1	E	105	GLU
1	E	106	THR
1	E	146	ASN
1	E	168	LYS
1	E	213	ARG
1	E	217	LYS
1	E	313	GLN
1	E	329	THR
1	E	364[A]	CYS
1	E	364[B]	CYS
1	E	382	ASN
1	E	394	LEU
1	E	527	ASN
1	E	669	LYS
1	F	20	ARG
1	F	48	LYS
1	F	84	LEU
1	F	109	LEU
1	F	148	MET
1	F	213	ARG
1	F	217	LYS
1	F	244	VAL
1	F	253	LYS
1	F	254	MET
1	F	300	GLU
1	F	313	GLN
1	F	357	ILE
1	F	359	VAL
1	F	360	LYS
1	F	531	VAL
1	F	576[A]	LYS
1	F	576[B]	LYS
1	F	633	LEU
1	F	660	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	66	GLN
1	A	70	GLN
1	A	146	ASN
1	A	257	ASN
1	A	263	ASN
1	A	313	GLN
1	A	452	ASN
1	A	527	ASN
1	A	529	ASN
1	A	578	ASN
1	A	611	ASN
1	B	66	GLN
1	B	70	GLN
1	B	113	GLN
1	B	286	HIS
1	B	313	GLN
1	B	361	ASN
1	B	366	HIS
1	B	450	ASN
1	B	452	ASN
1	B	527	ASN
1	B	529	ASN
1	B	578	ASN
1	B	611	ASN
1	C	23	HIS
1	C	113	GLN
1	C	146	ASN
1	C	263	ASN
1	C	313	GLN
1	C	348	HIS
1	C	361	ASN
1	C	452	ASN
1	C	527	ASN
1	C	529	ASN
1	C	611	ASN
1	D	288	ASN
1	D	313	GLN
1	D	366	HIS
1	D	450	ASN
1	D	452	ASN
1	D	527	ASN
1	D	529	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	611	ASN
1	E	23	HIS
1	E	70	GLN
1	E	113	GLN
1	E	146	ASN
1	E	149	HIS
1	E	263	ASN
1	E	286	HIS
1	E	313	GLN
1	E	348	HIS
1	E	361	ASN
1	E	366	HIS
1	E	452	ASN
1	E	527	ASN
1	E	529	ASN
1	E	571	ASN
1	E	611	ASN
1	F	70	GLN
1	F	113	GLN
1	F	288	ASN
1	F	313	GLN
1	F	348	HIS
1	F	366	HIS
1	F	450	ASN
1	F	452	ASN
1	F	527	ASN
1	F	529	ASN
1	F	571	ASN
1	F	611	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](#)

6 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	TYQ	F	405	1	13,14,15	2.55	2 (15%)	13,19,21	1.21	2 (15%)
1	TYQ	B	405	1	13,14,15	2.63	2 (15%)	13,19,21	1.55	3 (23%)
1	TYQ	E	405	1	13,14,15	2.30	2 (15%)	13,19,21	1.55	1 (7%)
1	TYQ	A	405	1	13,14,15	2.88	2 (15%)	13,19,21	1.53	4 (30%)
1	TYQ	C	405	1	13,14,15	2.91	2 (15%)	13,19,21	0.93	0
1	TYQ	D	405	1	13,14,15	2.71	2 (15%)	13,19,21	1.52	3 (23%)

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	TYQ	F	405	1	-	1/5/6/8	0/1/1/1
1	TYQ	B	405	1	-	1/5/6/8	0/1/1/1
1	TYQ	E	405	1	-	1/5/6/8	0/1/1/1
1	TYQ	A	405	1	-	1/5/6/8	0/1/1/1
1	TYQ	C	405	1	-	1/5/6/8	0/1/1/1
1	TYQ	D	405	1	-	1/5/6/8	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	405	TYQ	CE2-CZ	8.01	1.50	1.40
1	C	405	TYQ	CE2-CZ	7.72	1.49	1.40
1	F	405	TYQ	CE2-CZ	7.33	1.49	1.40
1	D	405	TYQ	CD1-CG	7.07	1.50	1.40
1	B	405	TYQ	CE2-CZ	6.90	1.48	1.40
1	C	405	TYQ	CD1-CG	6.85	1.49	1.40
1	E	405	TYQ	CE2-CZ	6.79	1.48	1.40
1	D	405	TYQ	CE2-CZ	6.32	1.48	1.40
1	A	405	TYQ	CD1-CG	6.21	1.48	1.40
1	B	405	TYQ	CD1-CG	6.06	1.48	1.40
1	F	405	TYQ	CD1-CG	5.07	1.47	1.40
1	E	405	TYQ	CD1-CG	4.46	1.46	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	405	TYQ	CB-CG-CD1	-4.08	116.41	121.05
1	D	405	TYQ	CD2-CG-CD1	3.57	122.28	118.18
1	A	405	TYQ	CB-CG-CD1	-3.54	117.03	121.05
1	B	405	TYQ	CD2-CG-CD1	2.86	121.47	118.18
1	B	405	TYQ	CB-CG-CD1	-2.83	117.84	121.05
1	F	405	TYQ	OH-CZ-CE2	2.74	121.00	116.50
1	B	405	TYQ	CE1-CZ-CE2	2.54	121.91	119.58
1	D	405	TYQ	CE1-CD1-CG	-2.49	117.68	120.75
1	F	405	TYQ	CD2-CG-CD1	2.28	120.80	118.18
1	D	405	TYQ	CE1-CZ-CE2	2.27	121.66	119.58
1	A	405	TYQ	CD2-CG-CD1	2.22	120.72	118.18
1	A	405	TYQ	OH-CZ-CE2	2.16	120.04	116.50
1	A	405	TYQ	CE1-CZ-CE2	2.01	121.42	119.58

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	405	TYQ	O-C-CA-CB
1	C	405	TYQ	O-C-CA-CB
1	E	405	TYQ	N-CA-CB-CG
1	F	405	TYQ	N-CA-CB-CG
1	A	405	TYQ	N-CA-CB-CG
1	D	405	TYQ	N-CA-CB-CG

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	405	TYQ	1	0
1	B	405	TYQ	2	0
1	E	405	TYQ	2	0
1	A	405	TYQ	6	0
1	C	405	TYQ	3	0
1	D	405	TYQ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 48 ligands modelled in this entry, 6 are monoatomic - leaving 42 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
2	GOL	A	706	-	5,5,5	0.48	0	5,5,5	0.54	0
2	GOL	E	705	-	5,5,5	0.49	0	5,5,5	1.41	0
2	GOL	F	702	-	5,5,5	0.44	0	5,5,5	0.47	0
2	GOL	E	704	-	5,5,5	0.36	0	5,5,5	0.74	0
2	GOL	A	703	-	5,5,5	0.45	0	5,5,5	0.38	0
2	GOL	E	703	-	5,5,5	0.34	0	5,5,5	0.56	0
2	GOL	F	704	-	5,5,5	0.38	0	5,5,5	0.58	0
2	GOL	C	703	-	5,5,5	0.29	0	5,5,5	0.70	0
4	PEO	F	707	3	1,1,1	0.05	0	-	-	-
5	NEH	E	707	-	2,2,2	0.87	0	0,1,1	-	-
5	NEH	C	708	-	2,2,2	0.48	0	0,1,1	-	-
5	NEH	D	706	-	2,2,2	0.64	0	0,1,1	-	-
2	GOL	C	702	-	5,5,5	0.26	0	5,5,5	1.29	0
2	GOL	B	701	-	5,5,5	0.87	0	5,5,5	0.70	0
2	GOL	D	704	-	5,5,5	0.35	0	5,5,5	0.63	0
2	GOL	C	704	-	5,5,5	0.50	0	5,5,5	0.36	0
2	GOL	C	705	-	5,5,5	0.61	0	5,5,5	0.64	0
5	NEH	A	708	-	2,2,2	0.78	0	0,1,1	-	-
2	GOL	B	706	-	5,5,5	0.28	0	5,5,5	0.84	0
5	NEH	B	709	-	2,2,2	0.58	0	0,1,1	-	-
2	GOL	B	703	-	5,5,5	0.51	0	5,5,5	0.84	0
2	GOL	D	705	-	5,5,5	0.45	0	5,5,5	0.19	0
2	GOL	B	710	-	5,5,5	0.29	0	5,5,5	0.57	0
2	GOL	E	702	-	5,5,5	0.37	0	5,5,5	0.94	0
2	GOL	B	705	-	5,5,5	0.35	0	5,5,5	0.55	0
4	PEO	B	708	3	1,1,1	0.36	0	-	-	-
4	PEO	A	707	3	1,1,1	0.02	0	-	-	-
2	GOL	A	705	-	5,5,5	0.44	0	5,5,5	0.70	0
2	GOL	C	707	-	5,5,5	0.55	0	5,5,5	0.70	0
2	GOL	B	704	-	5,5,5	0.45	0	5,5,5	0.62	0
2	GOL	D	703	-	5,5,5	0.59	0	5,5,5	0.65	0
2	GOL	F	706	-	5,5,5	0.34	0	5,5,5	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	C	706	-	5,5,5	0.31	0	5,5,5	0.55	0
2	GOL	F	703	-	5,5,5	0.42	0	5,5,5	0.42	0
2	GOL	F	705	-	5,5,5	0.30	0	5,5,5	1.12	0
2	GOL	B	707	-	5,5,5	0.47	0	5,5,5	0.54	0
4	PEO	E	706	3	1,1,1	0.08	0	-		
6	PO4	C	709	-	4,4,4	0.97	0	6,6,6	1.07	0
2	GOL	A	701	-	5,5,5	0.40	0	5,5,5	0.73	0
5	NEH	F	708	-	2,2,2	0.70	0	0,1,1	-	-
2	GOL	A	704	-	5,5,5	0.41	0	5,5,5	0.40	0
2	GOL	D	702	-	5,5,5	0.47	0	5,5,5	0.89	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
2	GOL	A	706	-	-	0/4/4/4	-
2	GOL	E	705	-	-	2/4/4/4	-
2	GOL	F	702	-	-	2/4/4/4	-
2	GOL	E	704	-	-	0/4/4/4	-
2	GOL	A	703	-	-	3/4/4/4	-
2	GOL	E	703	-	-	4/4/4/4	-
2	GOL	F	704	-	-	2/4/4/4	-
2	GOL	C	703	-	-	2/4/4/4	-
2	GOL	C	702	-	-	4/4/4/4	-
2	GOL	B	701	-	-	1/4/4/4	-
2	GOL	D	704	-	-	3/4/4/4	-
2	GOL	C	704	-	-	1/4/4/4	-
2	GOL	C	705	-	-	2/4/4/4	-
2	GOL	B	706	-	-	2/4/4/4	-
2	GOL	B	703	-	-	2/4/4/4	-
2	GOL	D	705	-	-	0/4/4/4	-
2	GOL	B	710	-	-	2/4/4/4	-
2	GOL	E	702	-	-	2/4/4/4	-
2	GOL	B	705	-	-	3/4/4/4	-
2	GOL	A	705	-	-	2/4/4/4	-
2	GOL	C	707	-	-	2/4/4/4	-
2	GOL	B	704	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	D	703	-	-	4/4/4/4	-
2	GOL	F	706	-	-	4/4/4/4	-
2	GOL	C	706	-	-	2/4/4/4	-
2	GOL	F	703	-	-	2/4/4/4	-
2	GOL	F	705	-	-	2/4/4/4	-
2	GOL	B	707	-	-	2/4/4/4	-
2	GOL	A	701	-	-	0/4/4/4	-
2	GOL	A	704	-	-	4/4/4/4	-
2	GOL	D	702	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	703	GOL	O1-C1-C2-C3
2	A	705	GOL	O1-C1-C2-O2
2	A	705	GOL	O1-C1-C2-C3
2	B	703	GOL	O1-C1-C2-C3
2	B	704	GOL	O1-C1-C2-C3
2	B	710	GOL	O1-C1-C2-C3
2	C	702	GOL	O1-C1-C2-O2
2	C	702	GOL	O1-C1-C2-C3
2	C	703	GOL	C1-C2-C3-O3
2	C	703	GOL	O2-C2-C3-O3
2	C	706	GOL	C1-C2-C3-O3
2	C	707	GOL	O1-C1-C2-O2
2	C	707	GOL	O1-C1-C2-C3
2	D	703	GOL	O1-C1-C2-C3
2	D	703	GOL	C1-C2-C3-O3
2	D	703	GOL	O2-C2-C3-O3
2	D	704	GOL	O1-C1-C2-C3
2	E	702	GOL	O1-C1-C2-C3
2	E	703	GOL	O1-C1-C2-C3
2	F	703	GOL	C1-C2-C3-O3
2	F	704	GOL	O1-C1-C2-C3
2	F	706	GOL	O1-C1-C2-C3
2	B	703	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	706	GOL	O2-C2-C3-O3
2	D	704	GOL	O1-C1-C2-O2
2	F	703	GOL	O2-C2-C3-O3
2	A	703	GOL	C1-C2-C3-O3
2	A	704	GOL	O1-C1-C2-C3
2	A	704	GOL	C1-C2-C3-O3
2	B	704	GOL	C1-C2-C3-O3
2	B	705	GOL	C1-C2-C3-O3
2	B	706	GOL	O1-C1-C2-C3
2	C	702	GOL	C1-C2-C3-O3
2	D	702	GOL	O1-C1-C2-C3
2	E	703	GOL	C1-C2-C3-O3
2	E	705	GOL	C1-C2-C3-O3
2	F	702	GOL	O1-C1-C2-C3
2	F	705	GOL	C1-C2-C3-O3
2	F	706	GOL	C1-C2-C3-O3
2	B	705	GOL	O2-C2-C3-O3
2	C	702	GOL	O2-C2-C3-O3
2	E	702	GOL	O1-C1-C2-O2
2	E	703	GOL	O1-C1-C2-O2
2	F	705	GOL	O2-C2-C3-O3
2	F	706	GOL	O1-C1-C2-O2
2	A	703	GOL	O1-C1-C2-O2
2	A	704	GOL	O1-C1-C2-O2
2	B	704	GOL	O1-C1-C2-O2
2	B	704	GOL	O2-C2-C3-O3
2	B	710	GOL	O1-C1-C2-O2
2	F	704	GOL	O1-C1-C2-O2
2	F	706	GOL	O2-C2-C3-O3
2	A	704	GOL	O2-C2-C3-O3
2	B	706	GOL	O1-C1-C2-O2
2	B	707	GOL	O2-C2-C3-O3
2	C	705	GOL	O1-C1-C2-O2
2	C	705	GOL	O2-C2-C3-O3
2	B	705	GOL	O1-C1-C2-O2
2	D	702	GOL	O2-C2-C3-O3
2	D	703	GOL	O1-C1-C2-O2
2	D	704	GOL	O2-C2-C3-O3
2	E	703	GOL	O2-C2-C3-O3
2	E	705	GOL	O2-C2-C3-O3
2	F	702	GOL	O1-C1-C2-O2
2	B	701	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	707	GOL	C1-C2-C3-O3
2	C	704	GOL	C1-C2-C3-O3

There are no ring outliers.

27 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	706	GOL	1	0
2	E	705	GOL	4	0
2	F	702	GOL	4	0
2	E	704	GOL	5	0
2	A	703	GOL	7	0
2	E	703	GOL	2	0
2	F	704	GOL	1	0
2	C	703	GOL	1	0
5	C	708	NEH	1	0
2	C	702	GOL	2	0
2	B	701	GOL	7	0
2	C	704	GOL	3	0
2	C	705	GOL	1	0
5	A	708	NEH	5	0
5	B	709	NEH	2	0
2	D	705	GOL	1	0
4	B	708	PEO	1	0
4	A	707	PEO	1	0
2	B	704	GOL	3	0
2	F	706	GOL	1	0
2	F	705	GOL	1	0
2	B	707	GOL	6	0
4	E	706	PEO	1	0
6	C	709	PO4	1	0
5	F	708	NEH	2	0
2	A	704	GOL	1	0
2	D	702	GOL	3	0

5.7 Other polymers [i](#)

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, 95th 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	653/692 (94%)	-0.59	6 (0%) 81 80	12, 29, 53, 88	13 (1%)
1	B	654/692 (94%)	-0.78	7 (1%) 78 77	13, 25, 46, 69	11 (1%)
1	C	654/692 (94%)	-0.64	6 (0%) 81 80	13, 30, 52, 85	12 (1%)
1	D	654/692 (94%)	-0.42	6 (0%) 81 80	14, 36, 59, 93	9 (1%)
1	E	653/692 (94%)	-0.58	7 (1%) 78 77	14, 30, 54, 87	18 (2%)
1	F	654/692 (94%)	-0.58	7 (1%) 78 77	13, 30, 55, 82	9 (1%)
All	All	3922/4152 (94%)	-0.60	39 (0%) 79 79	12, 30, 55, 93	72 (1%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	672	VAL	6.5
1	A	334	LEU	5.3
1	D	672	VAL	4.6
1	A	18	PRO	4.5
1	D	334	LEU	4.5
1	B	437	ASP	4.4
1	C	672	VAL	4.2
1	B	671	ALA	4.2
1	C	334	LEU	3.9
1	F	672	VAL	3.9
1	C	18	PRO	3.8
1	D	18	PRO	3.4
1	E	19	ALA	3.4
1	E	22	ALA	3.4
1	E	334	LEU	3.3
1	C	336[A]	CYS	3.2
1	E	336[A]	CYS	3.2
1	E	335	GLY	3.1
1	B	336[A]	CYS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	336	CYS	3.1
1	E	20	ARG	3.0
1	A	19	ALA	2.9
1	F	18	PRO	2.8
1	B	18	PRO	2.8
1	B	334	LEU	2.7
1	F	19	ALA	2.7
1	D	22	ALA	2.6
1	F	22	ALA	2.6
1	A	336	CYS	2.5
1	C	22	ALA	2.4
1	F	336	CYS	2.3
1	F	334	LEU	2.2
1	D	21	PRO	2.1
1	C	335	GLY	2.1
1	A	22	ALA	2.1
1	B	211[A]	ARG	2.1
1	A	20	ARG	2.1
1	B	335	GLY	2.1
1	F	335	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TYQ	C	405	14/15	0.94	0.08	27,35,43,45	0
1	TYQ	A	405	14/15	0.96	0.07	26,30,38,40	0
1	TYQ	D	405	14/15	0.96	0.07	35,39,42,43	0
1	TYQ	F	405	14/15	0.96	0.07	29,33,41,48	0
1	TYQ	E	405	14/15	0.97	0.06	21,24,41,44	0
1	TYQ	B	405	14/15	0.97	0.06	20,25,33,35	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	C	707	6/6	0.63	0.23	45,59,67,70	0
5	NEH	F	708	3/3	0.71	0.19	34,34,35,36	0
5	NEH	E	707	3/3	0.73	0.20	29,29,29,33	0
5	NEH	D	706	3/3	0.76	0.19	34,34,34,39	0
2	GOL	C	705	6/6	0.81	0.18	61,66,66,69	0
5	NEH	A	708	3/3	0.82	0.17	29,29,32,33	0
6	PO4	C	709	5/5	0.82	0.17	33,33,39,40	5
2	GOL	E	704	6/6	0.83	0.16	53,64,67,74	0
2	GOL	D	704	6/6	0.83	0.17	50,53,62,68	0
2	GOL	D	705	6/6	0.83	0.18	83,85,85,87	0
2	GOL	C	706	6/6	0.84	0.15	51,57,63,68	0
2	GOL	E	705	6/6	0.85	0.15	48,51,53,55	0
2	GOL	E	702	6/6	0.85	0.16	57,57,58,62	0
2	GOL	B	706	6/6	0.86	0.13	50,56,59,64	0
2	GOL	A	704	6/6	0.86	0.13	56,58,61,61	0
2	GOL	A	705	6/6	0.87	0.12	46,52,54,55	0
5	NEH	B	709	3/3	0.87	0.13	35,35,37,39	0
2	GOL	A	703	6/6	0.87	0.15	55,66,67,68	0
2	GOL	C	702	6/6	0.87	0.12	47,56,57,58	0
2	GOL	D	702	6/6	0.87	0.12	52,55,57,61	0
2	GOL	D	703	6/6	0.87	0.13	40,53,55,58	0
2	GOL	B	703	6/6	0.88	0.10	43,46,47,48	0
2	GOL	F	703	6/6	0.88	0.15	56,62,65,66	0
2	GOL	F	705	6/6	0.89	0.12	57,60,62,63	0
2	GOL	B	705	6/6	0.89	0.14	50,57,63,68	0
2	GOL	A	706	6/6	0.89	0.12	49,58,65,68	0
5	NEH	C	708	3/3	0.89	0.13	37,37,39,40	0
2	GOL	B	707	6/6	0.90	0.13	50,56,57,58	0
2	GOL	C	704	6/6	0.90	0.12	51,56,58,61	0
2	GOL	B	710	6/6	0.90	0.13	26,40,42,43	6
2	GOL	F	706	6/6	0.92	0.09	40,48,50,51	0
2	GOL	C	703	6/6	0.92	0.09	47,50,51,51	0
2	GOL	F	704	6/6	0.92	0.09	47,48,49,51	0
2	GOL	F	702	6/6	0.92	0.12	43,52,53,55	0
2	GOL	E	703	6/6	0.93	0.12	50,59,62,63	0
2	GOL	B	701	6/6	0.94	0.08	11,18,20,23	6
4	PEO	B	708	2/2	0.96	0.07	16,16,16,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	B	704	6/6	0.96	0.12	25,39,40,48	0
2	GOL	A	701	6/6	0.96	0.09	27,31,32,32	0
4	PEO	A	707	2/2	0.96	0.06	18,18,18,29	0
4	PEO	F	707	2/2	0.97	0.06	18,18,18,29	0
4	PEO	E	706	2/2	0.98	0.06	14,14,14,27	0
3	CU	D	701	1/1	0.99	0.02	29,29,29,29	0
3	CU	C	701	1/1	1.00	0.01	25,25,25,25	0
3	CU	A	702	1/1	1.00	0.01	21,21,21,21	0
3	CU	E	701	1/1	1.00	0.02	19,19,19,19	0
3	CU	F	701	1/1	1.00	0.02	23,23,23,23	0
3	CU	B	702	1/1	1.00	0.02	19,19,19,19	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.