



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:39 PM UTC

PDB ID : 3O4J / pdb_00003o4j
Title : Structure and Catalysis of Acylaminoacyl Peptidase
Authors : Harmat, V.; Domokos, K.; Menyhard, D.K.; Pallo, A.; Szeltner, Z.; Szamosi, I.; Beke-Somfai, T.; Naray-Szabo, G.; Polgar, L.
Deposited on : 2010-07-27
Resolution : 2.50 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

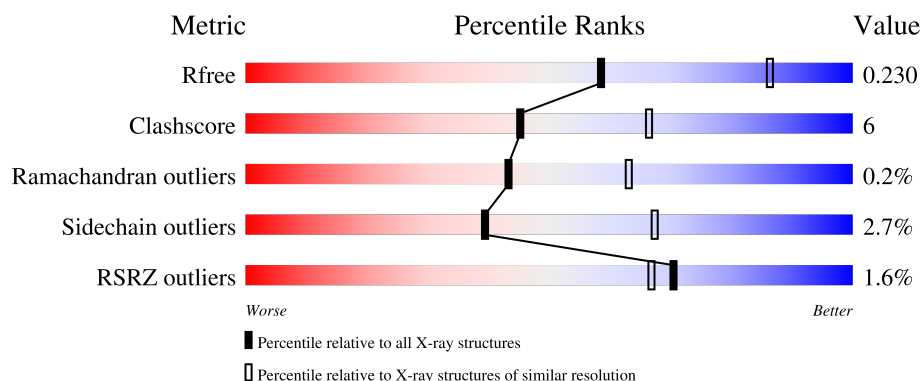
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	582	86%12%..
1	B	582	3% 86%11%..
1	C	582	84%14%..
1	D	582	3% 86%10%..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18121 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.

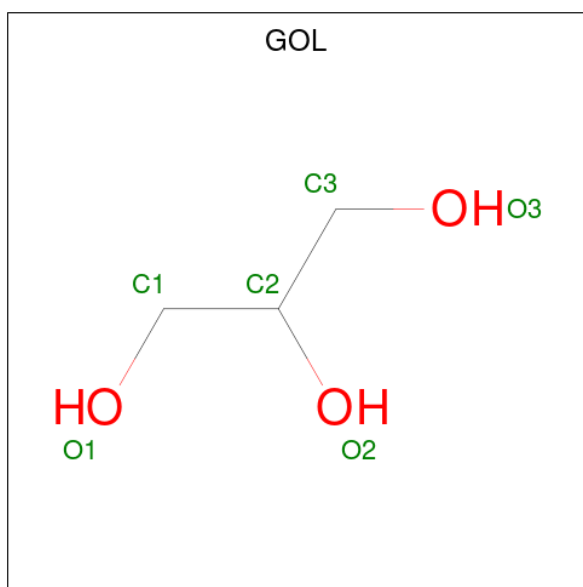
- Molecule 1 is a protein called Acylamino-acid-releasing enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	S	0	2	0
			4394	2778	773	831	12			
1	B	574	Total	C	N	O	S	0	2	0
			4357	2758	767	820	12			
1	C	579	Total	C	N	O	S	0	6	0
			4431	2803	779	836	13			
1	D	576	Total	C	N	O	S	0	5	0
			4371	2766	764	829	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	524	ASN	ASP	engineered mutation	UNP Q9YBQ2
B	524	ASN	ASP	engineered mutation	UNP Q9YBQ2
C	524	ASN	ASP	engineered mutation	UNP Q9YBQ2
D	524	ASN	ASP	engineered mutation	UNP Q9YBQ2

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



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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Cl	0	0
			2	2		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		

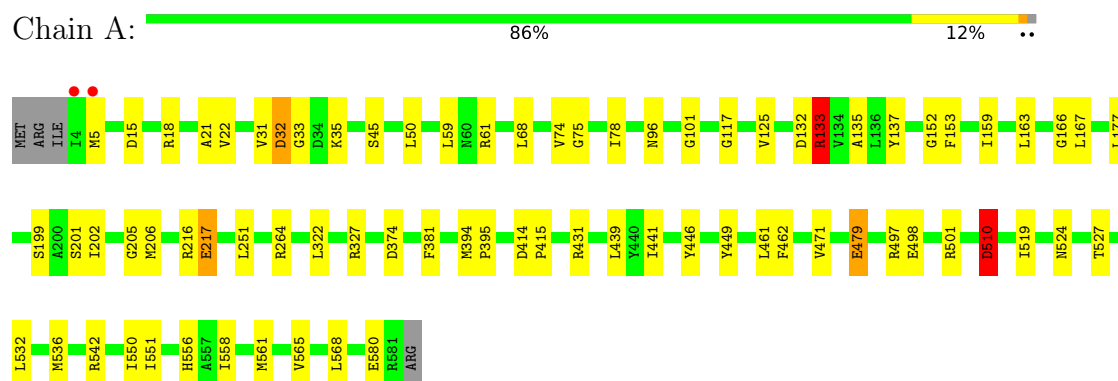
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	82	Total 82	O 82	0	0
5	B	180	Total 180	O 180	0	0
5	C	179	Total 179	O 179	0	0
5	D	94	Total 94	O 94	0	0

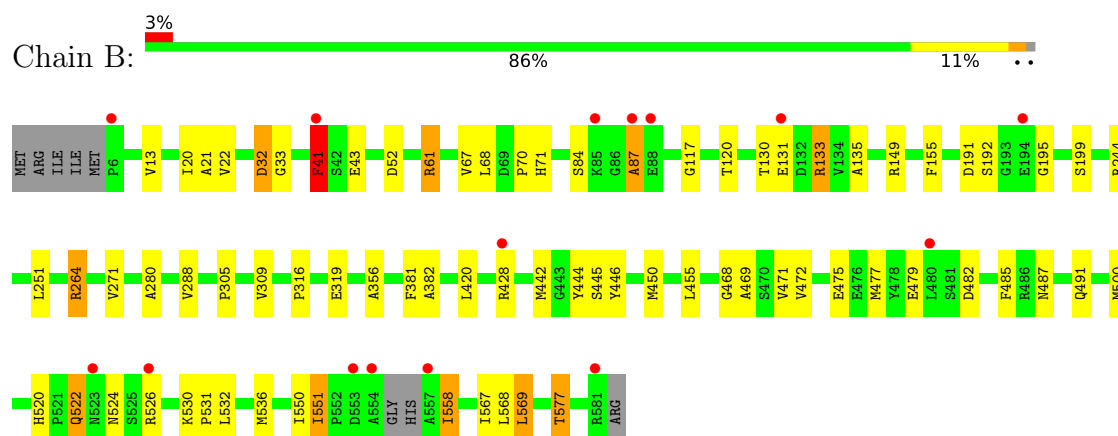
3 Residue-property plots

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.

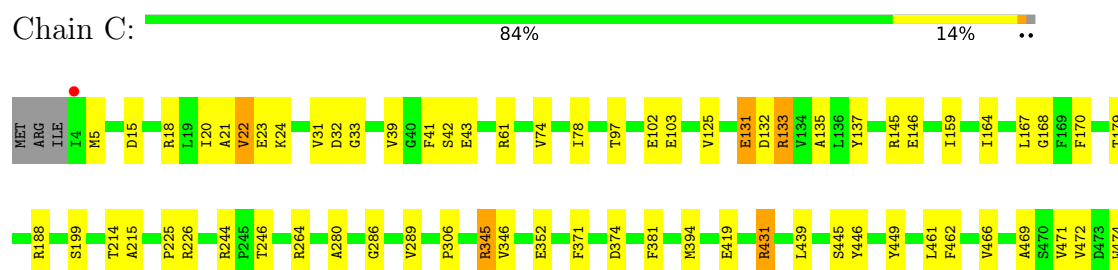
• Molecule 1: Acylamino-acid-releasing enzyme



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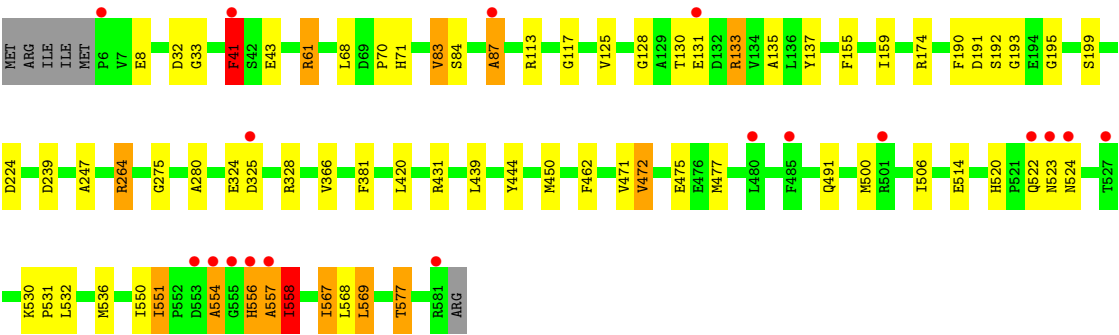
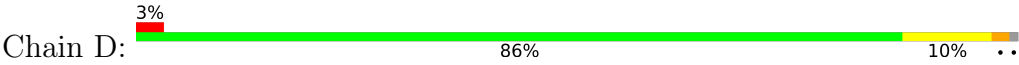


• Molecule 1: Acylamino-acid-releasing enzyme





● Molecule 1: Acylamino-acid-releasing enzyme



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.27Å 227.52Å 110.68Å 90.00° 100.37° 90.00°	Depositor
Resolution (Å)	29.52 – 2.50 29.52 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.9 (29.52-2.50) 96.8 (29.52-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.199 , 0.236 0.197 , 0.230	Depositor DCC
R_{free} test set	7760 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18121	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NA, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.11	3/4494 (0.1%)	1.02	3/6096 (0.0%)
1	B	1.40	14/4454 (0.3%)	1.08	12/6039 (0.2%)
1	C	1.38	14/4544 (0.3%)	1.08	9/6161 (0.1%)
1	D	1.26	10/4471 (0.2%)	1.07	7/6066 (0.1%)
All	All	1.29	41/17963 (0.2%)	1.06	31/24362 (0.1%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	444	TYR	CE1-CZ	-8.81	1.17	1.38
1	D	444	TYR	CG-CD2	-8.40	1.21	1.39
1	B	70	PRO	C-O	-8.24	1.14	1.23
1	D	444	TYR	CG-CD1	-7.69	1.23	1.39
1	B	444	TYR	CG-CD1	-7.50	1.23	1.39
1	C	78	ILE	C-O	-7.33	1.15	1.24
1	B	428	ARG	CB-CG	7.14	1.73	1.52
1	B	444	TYR	CG-CD2	-7.06	1.24	1.39
1	B	444	TYR	CE2-CZ	-7.04	1.21	1.38
1	A	510	ASP	CB-CG	-7.02	1.34	1.52
1	B	444	TYR	CE1-CZ	-6.97	1.21	1.38
1	D	280	ALA	CA-CB	-6.36	1.44	1.54
1	D	444	TYR	CE2-CZ	-6.25	1.23	1.38
1	C	286	GLY	C-O	-6.04	1.17	1.24
1	C	510	ASP	CB-CG	-5.83	1.37	1.52
1	C	551	ILE	CA-C	5.82	1.59	1.52
1	C	145	ARG	CA-C	-5.78	1.45	1.52
1	D	558	ILE	CA-CB	-5.67	1.46	1.54
1	B	280	ALA	CA-CB	-5.63	1.45	1.54
1	C	345	ARG	CD-NE	5.62	1.54	1.46
1	C	466	VAL	CA-CB	-5.57	1.47	1.54
1	B	319	GLU	C-O	-5.54	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	366	VAL	CA-CB	-5.51	1.47	1.54
1	D	70	PRO	C-O	-5.46	1.17	1.23
1	C	103	GLU	C-O	-5.44	1.17	1.24
1	C	23	GLU	N-CA	-5.39	1.39	1.46
1	B	442	MET	C-O	-5.37	1.17	1.23
1	D	569	LEU	C-O	-5.28	1.19	1.24
1	C	246	THR	C-O	-5.27	1.17	1.24
1	B	382	ALA	CA-CB	5.27	1.61	1.53
1	B	305	PRO	C-O	-5.20	1.20	1.25
1	B	135	ALA	C-O	-5.17	1.17	1.23
1	D	523	ASN	N-CA	5.12	1.51	1.46
1	C	102	GLU	N-CA	5.11	1.52	1.46
1	A	558	ILE	C-O	-5.11	1.18	1.24
1	C	289	VAL	CA-C	-5.10	1.46	1.52
1	B	67	VAL	C-O	-5.05	1.17	1.23
1	C	264	ARG	CA-C	-5.03	1.46	1.52
1	B	22	VAL	CA-CB	5.02	1.59	1.54
1	A	519	ILE	C-O	-5.01	1.18	1.24
1	C	39	VAL	C-O	-5.01	1.18	1.24

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	325	ASP	N-CA-CB	-8.03	98.43	110.07
1	A	133	ARG	N-CA-C	6.62	118.60	108.07
1	D	133	ARG	N-CA-C	6.30	117.88	107.73
1	D	41	PHE	CB-CA-C	-6.26	98.90	109.72
1	B	32	ASP	CB-CA-C	-6.00	107.97	115.89
1	B	558	ILE	N-CA-C	5.93	117.21	107.24
1	B	133	ARG	N-CA-C	5.93	117.28	107.73
1	C	280	ALA	CA-C-N	-5.89	113.87	119.76
1	C	280	ALA	C-N-CA	-5.89	113.87	119.76
1	D	8	GLU	CG-CD-OE1	5.78	131.69	118.40
1	D	554	ALA	N-CA-C	5.74	115.68	108.45
1	C	22	VAL	CB-CA-C	-5.60	102.27	111.51
1	B	120	THR	N-CA-C	-5.55	106.35	113.23
1	B	558	ILE	N-CA-CB	-5.46	105.11	112.10
1	C	133	ARG	N-CA-C	5.44	116.40	108.14
1	D	133	ARG	CG-CD-NE	5.42	123.93	112.00
1	C	562	GLU	CB-CG-CD	5.39	121.76	112.60
1	C	562	GLU	CA-CB-CG	-5.39	103.32	114.10
1	B	133	ARG	CG-CD-NE	5.36	123.79	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	356	ALA	CA-C-N	-5.29	115.31	120.98
1	B	356	ALA	C-N-CA	-5.29	115.31	120.98
1	B	244	ARG	CA-C-N	5.28	125.20	119.76
1	B	244	ARG	C-N-CA	5.28	125.20	119.76
1	C	504	SER	CA-C-N	5.26	125.07	119.28
1	C	504	SER	C-N-CA	5.26	125.07	119.28
1	A	32	ASP	CB-CA-C	-5.20	109.06	116.34
1	B	41	PHE	CB-CG-CD1	-5.12	111.99	120.70
1	C	346	VAL	N-CA-C	5.04	112.54	107.55
1	B	558	ILE	CA-CB-CG1	5.03	118.94	110.40
1	A	264	ARG	N-CA-C	5.02	116.70	109.07
1	D	224	ASP	CA-C-O	5.00	122.54	119.29

There are no chirality outliers.

There are no planarity outliers.

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	4394	0	4349	48	0
1	B	4357	0	4323	51	0
1	C	4431	0	4398	54	0
1	D	4371	0	4308	52	0
2	B	6	0	8	0	0
2	C	12	0	16	0	0
2	D	12	0	16	0	0
3	B	2	0	0	0	0
4	B	1	0	0	0	0
5	A	82	0	0	6	0
5	B	180	0	0	5	0
5	C	179	0	0	8	0
5	D	94	0	0	3	0
All	All	18121	0	17418	205	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 (205) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:556[B]:HIS:O	1:D:558:ILE:HG22	1.38	1.20
1:C:32:ASP:OD1	1:C:33:GLY:N	1.91	1.02
1:A:133:ARG:HH11	1:A:133:ARG:HG2	1.21	1.02
1:B:536:MET:HE1	1:B:550:ILE:HD11	1.39	1.02
1:D:556[B]:HIS:O	1:D:558:ILE:CG2	2.14	0.96
1:D:536:MET:HE1	1:D:550:ILE:HD11	1.48	0.95
1:B:475:GLU:HA	1:B:500:MET:HE3	1.54	0.90
1:B:32:ASP:CG	1:B:33:GLY:H	1.81	0.88
1:C:498:GLU:OE1	1:C:501[A]:ARG:NH2	2.09	0.86
1:C:226:ARG:HD2	5:C:770:HOH:O	1.75	0.85
1:C:199:SER:HB2	5:C:608:HOH:O	1.77	0.85
1:A:32:ASP:CG	1:A:33:GLY:H	1.86	0.83
1:D:32:ASP:CG	1:D:33:GLY:H	1.85	0.81
1:C:43[A]:GLU:OE1	5:C:756:HOH:O	1.97	0.81
1:C:32:ASP:CG	1:C:33:GLY:H	1.86	0.81
1:D:475:GLU:HA	1:D:500:MET:HE3	1.62	0.80
1:A:31:VAL:HG22	1:A:74:VAL:O	1.81	0.79
1:D:125:VAL:HG21	1:D:159:ILE:CD1	2.13	0.79
1:B:482:ASP:OD2	1:B:526:ARG:NH1	2.19	0.76
1:B:41:PHE:CD2	1:B:41:PHE:N	2.55	0.75
1:A:439:LEU:HD12	5:A:683:HOH:O	1.89	0.73
1:C:188:ARG:NH1	1:C:225:PRO:O	2.21	0.73
1:A:15:ASP:OD1	1:A:18:ARG:NH2	2.22	0.72
1:C:31[A]:VAL:HG13	1:C:74:VAL:O	1.90	0.72
1:B:41:PHE:N	1:B:41:PHE:HD2	1.88	0.70
1:A:163:LEU:HD23	1:A:202:ILE:HD13	1.74	0.69
1:B:32:ASP:CG	1:B:33:GLY:N	2.49	0.69
1:C:15:ASP:OD1	1:C:18:ARG:NH2	2.26	0.69
1:A:217:GLU:N	1:A:217:GLU:OE2	2.27	0.67
1:A:133:ARG:HG2	1:A:133:ARG:NH1	1.97	0.67
1:D:471:VAL:HG22	1:D:477:MET:HE2	1.78	0.66
1:D:551:ILE:HD13	1:D:551:ILE:N	2.11	0.66
1:B:61:ARG:HH11	1:B:61:ARG:HG2	1.62	0.64
1:D:558:ILE:HG21	1:D:567:ILE:HD11	1.78	0.64
1:D:125:VAL:HB	1:D:159:ILE:HD11	1.80	0.63
1:B:133:ARG:HD2	1:B:149:ARG:HE	1.64	0.63
1:C:477:MET:HE3	1:C:489:ILE:HD11	1.80	0.62
1:B:520:HIS:CG	1:B:532:LEU:HD22	2.35	0.62
1:C:42:SER:O	1:C:43[B]:GLU:HG2	2.00	0.62
1:D:125:VAL:HG21	1:D:159:ILE:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:LEU:HD22	1:B:117:GLY:HA3	1.81	0.61
1:D:558:ILE:CG2	1:D:567:ILE:HD11	2.30	0.61
1:D:520:HIS:CG	1:D:532:LEU:HD22	2.36	0.60
1:D:551:ILE:HD13	1:D:551:ILE:H	1.66	0.60
1:B:20:ILE:HG22	1:B:43:GLU:HG2	1.83	0.60
1:D:125:VAL:CB	1:D:159:ILE:HD11	2.32	0.60
1:C:20:ILE:HG22	1:C:561:MET:SD	2.42	0.60
1:D:125:VAL:CG2	1:D:159:ILE:CD1	2.80	0.60
1:C:21:ALA:HB2	1:C:561:MET:HE1	1.84	0.59
1:D:192:SER:HB3	1:D:195:GLY:O	2.02	0.59
1:D:61:ARG:HG2	1:D:61:ARG:HH11	1.67	0.59
1:A:327:ARG:NH2	5:A:598:HOH:O	2.35	0.59
1:D:381:PHE:CD2	1:D:568:LEU:HD13	2.37	0.59
1:C:474:TRP:CZ3	1:C:477:MET:HE1	2.38	0.58
1:B:61:ARG:HG2	1:B:61:ARG:NH1	2.18	0.58
1:A:163:LEU:HD23	1:A:202:ILE:HG21	1.84	0.58
1:B:477:MET:HE3	1:B:485:PHE:HE1	1.69	0.58
1:D:32:ASP:CG	1:D:33:GLY:N	2.56	0.58
1:D:68:LEU:HD22	1:D:117:GLY:HA3	1.86	0.58
1:A:167:LEU:HD11	1:A:199:SER:HA	1.86	0.57
1:B:420:LEU:HA	1:B:450:MET:HE1	1.86	0.57
1:C:131:GLU:HG2	5:C:604:HOH:O	2.03	0.57
1:B:536:MET:CE	1:B:550:ILE:HD11	2.25	0.57
1:D:61:ARG:HG2	1:D:61:ARG:NH1	2.19	0.56
1:B:487:ASN:HB2	5:B:681:HOH:O	2.05	0.56
1:B:471:VAL:HG22	1:B:477:MET:HE2	1.88	0.55
5:A:611:HOH:O	1:B:577:THR:HG21	2.06	0.55
1:C:532:LEU:HD23	1:C:536:MET:CE	2.37	0.55
1:C:31[A]:VAL:CG1	1:C:97:THR:HG21	2.37	0.54
1:D:536:MET:CE	1:D:550:ILE:HD11	2.31	0.54
1:D:475:GLU:HA	1:D:500:MET:CE	2.35	0.54
1:C:536:MET:HE1	1:C:550:ILE:HD11	1.90	0.53
1:D:475:GLU:HG3	1:D:500:MET:HE2	1.90	0.53
1:A:498:GLU:OE1	1:A:501:ARG:NH1	2.30	0.53
5:A:611:HOH:O	1:B:577:THR:CG2	2.55	0.53
1:A:68:LEU:HD22	1:A:117:GLY:HA3	1.91	0.53
1:D:41:PHE:N	1:D:41:PHE:CD2	2.76	0.53
1:A:381:PHE:CD1	1:A:568:LEU:HD13	2.44	0.53
1:C:168:GLY:HA3	1:C:170:PHE:CE2	2.44	0.52
1:B:264:ARG:HD2	5:B:702:HOH:O	2.09	0.52
1:B:41:PHE:CE1	5:B:729:HOH:O	2.54	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:PHE:CD2	1:B:568:LEU:HD13	2.45	0.52
1:B:551:ILE:H	1:B:551:ILE:HD13	1.74	0.52
1:C:371:PHE:HB2	5:C:657:HOH:O	2.08	0.52
1:C:167:LEU:HD11	1:C:199:SER:HA	1.91	0.52
1:C:461:LEU:HD23	1:C:462:PHE:CE1	2.46	0.51
1:A:524:ASN:ND2	1:A:556[B]:HIS:ND1	2.52	0.51
1:B:84:SER:OG	1:B:87:ALA:HB2	2.11	0.51
1:C:31[A]:VAL:CG1	1:C:32:ASP:N	2.72	0.51
1:B:530:LYS:HB3	1:B:531:PRO:HD3	1.93	0.50
1:C:61:ARG:HD3	5:C:690:HOH:O	2.09	0.50
1:D:83:VAL:CG1	1:D:83:VAL:O	2.58	0.50
1:D:84:SER:OG	1:D:87:ALA:HB2	2.12	0.50
1:D:192:SER:CB	1:D:195:GLY:O	2.60	0.50
1:B:21:ALA:HA	1:B:43:GLU:HG3	1.93	0.50
1:C:381:PHE:CD1	1:C:568:LEU:HD13	2.47	0.50
1:D:556[B]:HIS:O	1:D:557[B]:ALA:C	2.55	0.50
1:A:32:ASP:CG	1:A:33:GLY:N	2.58	0.50
1:A:166:GLY:O	1:A:177:LEU:HD12	2.12	0.50
1:C:474:TRP:CE3	1:C:477:MET:HE2	2.47	0.50
1:C:431[B]:ARG:CZ	1:C:439:LEU:HD12	2.41	0.49
1:B:551:ILE:HD13	1:B:551:ILE:N	2.26	0.49
1:D:558:ILE:CG1	1:D:558:ILE:O	2.60	0.49
1:A:216:ARG:N	1:A:217:GLU:OE2	2.36	0.49
1:A:395:PRO:HD2	5:A:602:HOH:O	2.12	0.49
1:C:226:ARG:CD	5:C:770:HOH:O	2.45	0.49
1:C:474:TRP:CZ3	1:C:477:MET:CE	2.96	0.48
1:D:174:ARG:NE	1:D:193:GLY:O	2.46	0.48
1:B:61:ARG:HH11	1:B:61:ARG:CG	2.26	0.48
1:D:577:THR:CG2	5:D:665:HOH:O	2.62	0.48
1:A:374:ASP:CG	1:A:394:MET:HB3	2.39	0.48
1:D:130:THR:O	1:D:131:GLU:C	2.56	0.47
1:D:61:ARG:HH11	1:D:61:ARG:CG	2.27	0.47
1:C:168:GLY:HA3	1:C:170:PHE:CZ	2.50	0.47
1:B:191:ASP:HB3	5:B:727:HOH:O	2.14	0.47
1:B:420:LEU:CD1	1:B:450:MET:HE1	2.45	0.47
1:A:68:LEU:HD12	1:A:78:ILE:HG21	1.97	0.47
1:A:163:LEU:CD2	1:A:202:ILE:HD13	2.42	0.47
1:B:477:MET:HE3	1:B:485:PHE:CE1	2.49	0.47
1:D:239:ASP:HB2	1:D:275:GLY:O	2.14	0.47
1:B:477:MET:CE	1:B:485:PHE:HE1	2.29	0.46
1:C:31[A]:VAL:HG11	1:C:97:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:ALA:HB3	1:D:137:TYR:CE1	2.50	0.46
1:A:251:LEU:C	1:A:251:LEU:HD12	2.41	0.46
1:A:551:ILE:N	1:A:551:ILE:HD12	2.30	0.46
1:A:536:MET:HE1	1:A:550:ILE:HD11	1.97	0.46
1:B:524:ASN:OD1	1:B:524:ASN:C	2.59	0.46
1:A:32:ASP:OD2	1:A:35:LYS:HE3	2.15	0.45
1:C:474:TRP:CE3	1:C:477:MET:CE	3.00	0.45
1:D:524:ASN:OD1	1:D:524:ASN:C	2.60	0.45
1:C:41:PHE:CD2	1:C:41:PHE:C	2.95	0.45
1:A:135:ALA:HB3	1:A:137:TYR:CE1	2.52	0.45
1:C:374:ASP:CG	1:C:394:MET:HB3	2.41	0.45
1:B:199:SER:HB2	5:B:662:HOH:O	2.16	0.45
1:D:530:LYS:HB3	1:D:531:PRO:HD3	1.98	0.45
1:A:5:MET:N	1:A:580:GLU:OE2	2.49	0.45
1:C:526:ARG:NH1	1:C:556[A]:HIS:CE1	2.85	0.45
1:C:24:LYS:HG2	1:C:306:PRO:HD2	1.99	0.44
1:C:31[A]:VAL:HG12	1:C:32:ASP:N	2.30	0.44
1:A:21:ALA:HB2	1:A:561:MET:HE1	1.98	0.44
1:A:22:VAL:HG11	1:A:322:LEU:CD2	2.47	0.44
1:B:522:GLN:HE21	1:B:522:GLN:HB2	1.54	0.44
1:C:345:ARG:HD2	5:C:605:HOH:O	2.16	0.44
1:D:431:ARG:HH11	1:D:439:LEU:HD12	1.82	0.44
1:A:50:LEU:HG	1:A:59:LEU:HD21	1.99	0.44
1:A:510:ASP:OD1	1:A:542:ARG:HD3	2.18	0.44
1:A:152:GLY:O	1:A:153:PHE:C	2.61	0.44
1:A:479:GLU:OE2	5:A:604:HOH:O	2.21	0.44
1:B:475:GLU:HG3	1:B:500:MET:HE2	2.00	0.44
1:A:61:ARG:NE	1:A:101:GLY:O	2.50	0.44
1:A:471:VAL:HG22	1:A:527:THR:HG22	1.99	0.43
1:A:22:VAL:O	1:A:22:VAL:HG23	2.18	0.43
1:D:577:THR:HG21	5:D:665:HOH:O	2.17	0.43
1:A:132:ASP:OD2	1:A:133:ARG:NH1	2.52	0.43
1:C:446:TYR:O	1:C:449:TYR:HB3	2.19	0.43
1:A:446:TYR:O	1:A:449:TYR:HB3	2.19	0.43
1:C:41:PHE:C	1:C:41:PHE:HD2	2.27	0.43
1:C:526:ARG:CZ	1:C:556[A]:HIS:ND1	2.82	0.43
1:A:414:ASP:N	1:A:415:PRO:CD	2.82	0.43
1:B:468:GLY:O	1:B:469:ALA:C	2.62	0.43
1:D:558:ILE:HG21	1:D:558:ILE:HD13	1.75	0.42
1:A:75:GLY:O	1:A:96[A]:ASN:ND2	2.51	0.42
1:B:130:THR:O	1:B:131:GLU:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:SER:HB3	1:B:195:GLY:O	2.19	0.42
1:C:472:VAL:HG12	1:C:506:ILE:HB	2.01	0.42
1:A:125:VAL:HB	1:A:159:ILE:HD11	2.01	0.42
1:D:113:ARG:O	1:D:128:GLY:HA2	2.19	0.42
1:D:554:ALA:HB1	1:D:567:ILE:CG2	2.49	0.42
1:A:561:MET:O	1:A:565:VAL:HG23	2.19	0.42
1:B:309:VAL:HG12	1:B:316:PRO:HA	2.02	0.42
1:B:155:PHE:CD1	1:B:155:PHE:N	2.88	0.42
1:D:462:PHE:O	1:D:514:GLU:HG2	2.20	0.42
1:A:441:ILE:HD12	1:A:462:PHE:CE1	2.55	0.42
1:C:445:SER:HA	1:C:469:ALA:O	2.18	0.42
1:D:420:LEU:HB2	1:D:450:MET:HE1	2.01	0.42
1:C:479:GLU:H	1:C:479:GLU:HG2	1.74	0.42
1:C:164:ILE:O	1:C:179:THR:HA	2.20	0.41
1:D:472:VAL:HG13	1:D:506:ILE:HB	2.01	0.41
1:C:135:ALA:HB3	1:C:137:TYR:CE1	2.55	0.41
1:C:475:GLU:O	1:C:479:GLU:HG2	2.20	0.41
1:B:13:VAL:HG22	1:B:569:LEU:HD21	2.01	0.41
1:D:247:ALA:HB3	1:D:264:ARG:HG3	2.01	0.41
1:B:52:ASP:C	1:B:52:ASP:OD1	2.61	0.41
1:C:5:MET:HB3	1:C:580:GLU:OE2	2.21	0.41
1:C:214:THR:O	1:C:215:ALA:C	2.63	0.41
1:C:532:LEU:HD23	1:C:536:MET:HE2	2.02	0.41
1:A:532:LEU:HD23	1:A:536:MET:CE	2.50	0.41
1:D:190:PHE:CD1	1:D:190:PHE:N	2.89	0.41
1:A:251:LEU:HD12	1:A:251:LEU:O	2.20	0.41
1:B:475:GLU:HG3	1:B:500:MET:CE	2.51	0.41
1:B:569:LEU:HD12	1:B:569:LEU:HA	1.89	0.41
1:D:199:SER:HB2	5:D:612:HOH:O	2.20	0.41
1:B:251:LEU:C	1:B:251:LEU:HD12	2.45	0.41
1:B:445:SER:OG	1:B:446:TYR:N	2.52	0.41
1:A:461:LEU:HD23	1:A:462:PHE:CE1	2.56	0.41
1:C:133:ARG:NH2	1:C:146:GLU:OE1	2.51	0.41
1:C:471:VAL:HG22	1:C:527:THR:HG22	2.02	0.40
1:D:324:GLU:HG2	1:D:328:ARG:NH1	2.36	0.40
1:A:205:GLY:O	1:A:206:MET:HB2	2.20	0.40
1:B:192:SER:CB	1:B:195:GLY:O	2.68	0.40
1:C:125:VAL:HB	1:C:159:ILE:HD11	2.03	0.40
1:B:271:VAL:HG13	1:B:288:VAL:HG21	2.02	0.40
1:B:420:LEU:HD13	1:B:450:MET:HE1	2.03	0.40
1:D:155:PHE:CD1	1:D:155:PHE:N	2.89	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	578/582 (99%)	560 (97%)	18 (3%)	0	100	100
1	B	572/582 (98%)	550 (96%)	21 (4%)	1 (0%)	43	63
1	C	583/582 (100%)	566 (97%)	17 (3%)	0	100	100
1	D	579/582 (100%)	550 (95%)	24 (4%)	5 (1%)	14	27
All	All	2312/2328 (99%)	2226 (96%)	80 (4%)	6 (0%)	43	55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	557[A]	ALA
1	D	557[B]	ALA
1	B	87	ALA
1	D	556[A]	HIS
1	D	556[B]	HIS
1	D	87	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	460/469 (98%)	452 (98%)	8 (2%)	53	78
1	B	454/469 (97%)	440 (97%)	14 (3%)	35	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	465/469 (99%)	453 (97%)	12 (3%)	40	68
1	D	453/469 (97%)	436 (96%)	17 (4%)	29	56
All	All	1832/1876 (98%)	1781 (97%)	51 (3%)	39	66

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	SER
1	A	133	ARG
1	A	201	SER
1	A	217	GLU
1	A	431	ARG
1	A	479	GLU
1	A	497	ARG
1	A	510	ASP
1	B	41	PHE
1	B	61	ARG
1	B	71	HIS
1	B	264	ARG
1	B	455	LEU
1	B	472	VAL
1	B	479	GLU
1	B	491	GLN
1	B	522	GLN
1	B	551	ILE
1	B	558	ILE
1	B	567	ILE
1	B	569	LEU
1	B	577	THR
1	C	22	VAL
1	C	131	GLU
1	C	132	ASP
1	C	244	ARG
1	C	352	GLU
1	C	419	GLU
1	C	431[A]	ARG
1	C	431[B]	ARG
1	C	479	GLU
1	C	497	ARG
1	C	532	LEU
1	C	567	ILE

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Mol	Chain	Res	Type
1	D	41	PHE
1	D	43[A]	GLU
1	D	43[B]	GLU
1	D	61	ARG
1	D	71	HIS
1	D	83	VAL
1	D	133	ARG
1	D	191	ASP
1	D	264	ARG
1	D	472	VAL
1	D	491	GLN
1	D	522	GLN
1	D	551	ILE
1	D	558	ILE
1	D	567	ILE
1	D	569	LEU
1	D	577	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	B	28	GLN
1	B	89	GLN
1	B	282	GLN
1	B	522	GLN
1	C	28	GLN
1	D	28	GLN
1	D	89	GLN
1	D	522	GLN
1	D	559	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	D	583	-	5,5,5	0.76	0	5,5,5	0.73	0
2	GOL	C	583	-	5,5,5	0.94	0	5,5,5	0.59	0
2	GOL	D	584	-	5,5,5	0.75	0	5,5,5	1.47	1 (20%)
2	GOL	B	583	-	5,5,5	0.66	0	5,5,5	1.33	1 (20%)
2	GOL	C	584	-	5,5,5	0.69	0	5,5,5	0.81	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	D	583	-	-	4/4/4/4	-
2	GOL	C	583	-	-	2/4/4/4	-
2	GOL	D	584	-	-	0/4/4/4	-
2	GOL	B	583	-	-	4/4/4/4	-
2	GOL	C	584	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	583	GOL	O2-C2-C1	-2.23	99.94	109.18
2	D	584	GOL	O3-C3-C2	2.09	119.77	110.38

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	583	GOL	C1-C2-C3-O3
2	C	583	GOL	C1-C2-C3-O3
2	C	584	GOL	C1-C2-C3-O3
2	D	583	GOL	O1-C1-C2-C3
2	D	583	GOL	C1-C2-C3-O3
2	B	583	GOL	O2-C2-C3-O3
2	C	584	GOL	O2-C2-C3-O3
2	D	583	GOL	O1-C1-C2-O2
2	C	583	GOL	O2-C2-C3-O3
2	D	583	GOL	O2-C2-C3-O3
2	B	583	GOL	O1-C1-C2-O2
2	B	583	GOL	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	578/582 (99%)	-0.23	2 (0%) 90 87	21, 48, 71, 91	2 (0%)
1	B	574/582 (98%)	-0.27	15 (2%) 57 52	19, 36, 58, 67	2 (0%)
1	C	579/582 (99%)	-0.50	2 (0%) 90 87	17, 33, 45, 65	6 (1%)
1	D	576/582 (98%)	-0.08	18 (3%) 51 47	26, 44, 62, 80	5 (0%)
All	All	2307/2328 (99%)	-0.27	37 (1%) 70 67	17, 40, 63, 91	15 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	557	ALA	9.2
1	D	556[A]	HIS	9.0
1	D	555[A]	GLY	6.5
1	D	554	ALA	5.0
1	D	557[A]	ALA	4.0
1	D	523	ASN	4.0
1	A	4	ILE	3.7
1	D	41	PHE	3.6
1	B	553	ASP	3.4
1	B	554	ALA	3.4
1	B	85	LYS	3.4
1	D	501[A]	ARG	3.1
1	D	480	LEU	3.0
1	B	41	PHE	3.0
1	D	553	ASP	3.0
1	C	4	ILE	2.9
1	D	6	PRO	2.9
1	B	526	ARG	2.9
1	B	131	GLU	2.7
1	D	325	ASP	2.7
1	B	88	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	428	ARG	2.5
1	B	480	LEU	2.5
1	D	485	PHE	2.4
1	D	524	ASN	2.4
1	D	131	GLU	2.4
1	C	582	ARG	2.3
1	A	5	MET	2.3
1	D	527	THR	2.3
1	D	87	ALA	2.2
1	D	581	ARG	2.2
1	B	6	PRO	2.2
1	B	523	ASN	2.2
1	D	522	GLN	2.2
1	B	194	GLU	2.2
1	B	581	ARG	2.2
1	B	87	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no 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	583	6/6	0.76	0.14	51,55,57,59	0
2	GOL	C	584	6/6	0.86	0.16	49,51,52,53	0
2	GOL	D	583	6/6	0.90	0.13	49,56,58,58	0
2	GOL	D	584	6/6	0.93	0.11	42,48,49,50	0
2	GOL	B	583	6/6	0.94	0.09	44,45,47,51	0
3	CL	B	584	1/1	0.96	0.19	46,46,46,46	0
4	NA	B	586	1/1	0.96	0.06	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	B	585	1/1	0.98	0.11	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.