Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2023 – 03:09 AM EDT

PDB ID	:	3O4G
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 (i) 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 (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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	Percentile Ranks	Value
Rfree		0.261
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		2.5%
RSRZ outliers		2.0%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
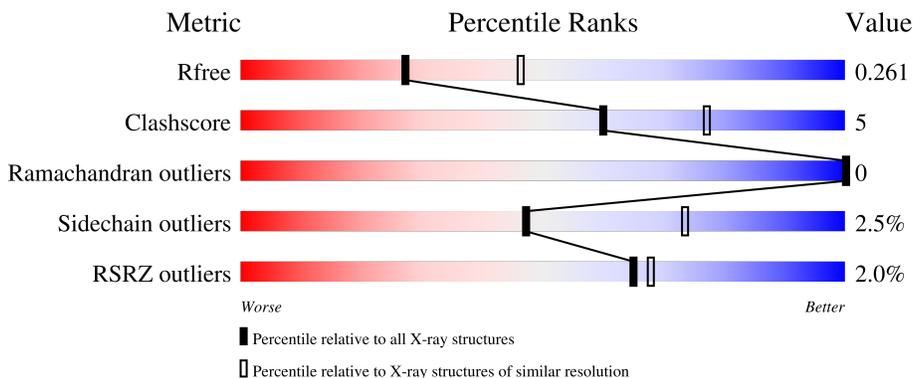
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	% 89% 10% ·
1	B	582	3% 87% 11% ··
1	C	582	% 90% 8% ·
1	D	582	4% 85% 12% ··

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 17523 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	577	Total	C	N	O	S	0	0	0
			4338	2751	753	822	12			
1	B	574	Total	C	N	O	S	0	0	0
			4243	2695	737	799	12			
1	C	576	Total	C	N	O	S	0	0	0
			4324	2741	750	821	12			
1	D	576	Total	C	N	O	S	0	0	0
			4254	2700	736	806	12			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
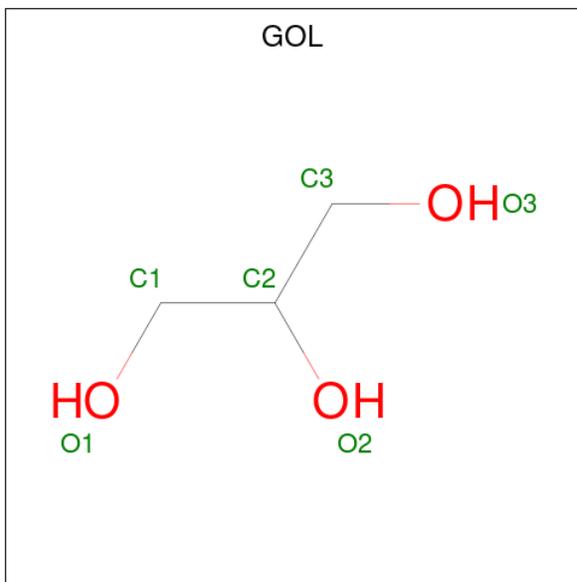
GOL

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

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

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	112	Total 112	O 112	0	0
3	B	73	Total 73	O 73	0	0
3	C	81	Total 81	O 81	0	0
3	D	74	Total 74	O 74	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
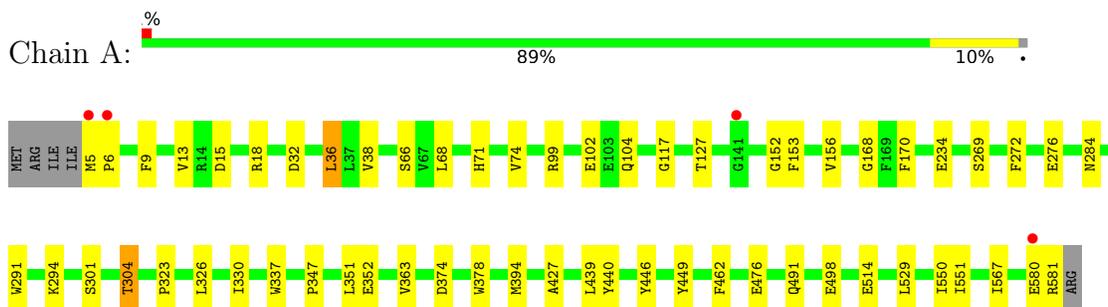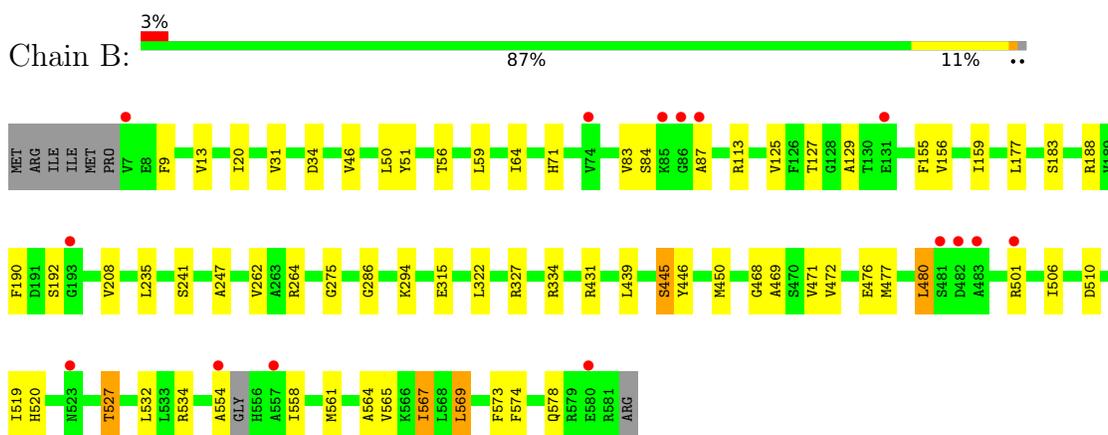
• Molecule 1: Acylamino-acid-releasing enzyme

• Molecule 1: Acylamino-acid-releasing enzyme

• Molecule 1: Acylamino-acid-releasing enzyme

Chain D:
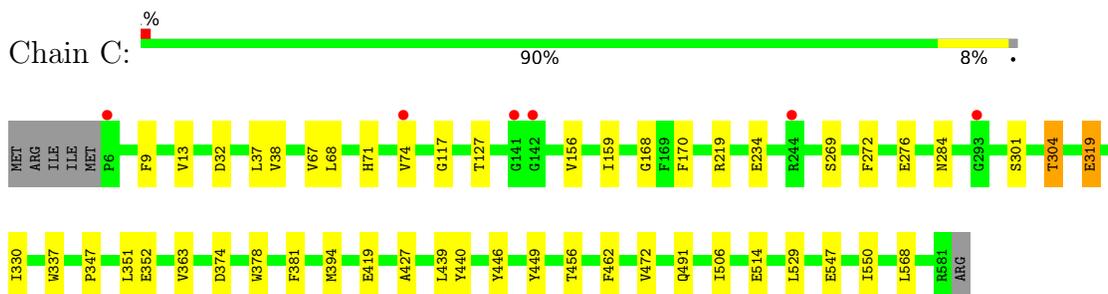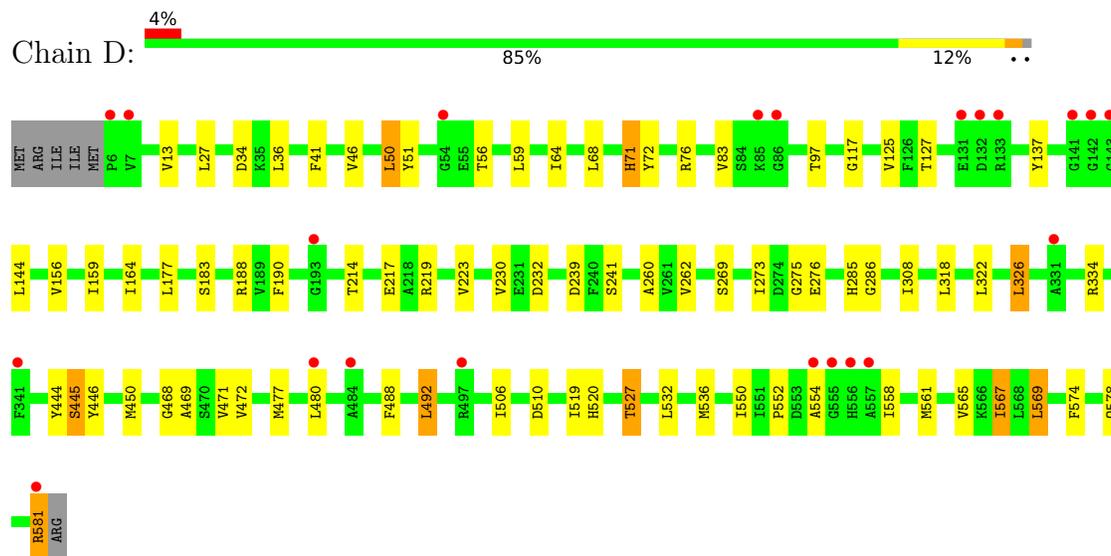
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	71.21Å 97.02Å 109.49Å 89.01° 109.20° 100.21°	Depositor
Resolution (Å)	19.64 – 2.50 19.64 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.4 (19.64-2.50) 94.4 (19.64-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.215 , 0.262 0.216 , 0.261	Depositor DCC
R_{free} test set	4439 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.0	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,h+l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17523	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.49	0/4431	0.63	0/6013
1	B	0.47	0/4331	0.63	0/5882
1	C	0.49	0/4417	0.64	0/5995
1	D	0.48	0/4345	0.63	0/5908
All	All	0.48	0/17524	0.63	0/23798

There are no bond length outliers.

There are no bond angle outliers.

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	4338	0	4275	34	0
1	B	4243	0	4149	44	0
1	C	4324	0	4258	26	0
1	D	4254	0	4142	57	0
2	A	12	0	16	3	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0
3	A	112	0	0	1	0
3	B	73	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	81	0	0	1	0
3	D	74	0	0	0	0
All	All	17523	0	16856	157	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 (157) 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:127:THR:HG23	1:D:156:VAL:HG23	1.61	0.82
1:C:71:HIS:HE1	1:C:159:ILE:O	1.64	0.79
1:A:9:PHE:O	1:A:13:VAL:HG23	1.83	0.78
1:A:127:THR:HG23	1:A:156:VAL:HG23	1.65	0.78
1:B:127:THR:HG23	1:B:156:VAL:HG23	1.69	0.75
1:C:127:THR:HG23	1:C:156:VAL:HG23	1.68	0.74
1:C:363:VAL:HG22	1:C:440:TYR:HB2	1.70	0.74
1:D:554:ALA:HB1	1:D:567:ILE:HD11	1.70	0.73
1:C:9:PHE:O	1:C:13:VAL:HG23	1.89	0.73
1:B:247:ALA:HB3	1:B:264:ARG:HB2	1.75	0.69
1:C:68:LEU:HD22	1:C:117:GLY:HA3	1.75	0.67
1:A:330:ILE:HG23	1:A:351:LEU:HD22	1.77	0.67
1:D:36:LEU:HD12	1:D:51:TYR:HD2	1.60	0.66
1:B:472:VAL:HG12	1:B:506:ILE:HB	1.77	0.66
1:C:71:HIS:CE1	1:C:159:ILE:O	2.47	0.66
1:A:5:MET:N	1:A:6:PRO:HD3	2.12	0.65
1:B:554:ALA:HB1	1:B:567:ILE:HD11	1.79	0.65
1:D:472:VAL:HG12	1:D:506:ILE:HB	1.77	0.65
1:B:520:HIS:CG	1:B:532:LEU:HD22	2.33	0.64
1:B:125:VAL:HG11	1:B:159:ILE:HD11	1.81	0.63
1:A:68:LEU:HD22	1:A:117:GLY:HA3	1.79	0.63
1:B:558:ILE:HG23	1:B:558:ILE:O	1.99	0.62
1:D:471:VAL:HG13	1:D:477:MET:SD	2.41	0.61
1:B:445:SER:OG	1:B:446:TYR:N	2.33	0.61
1:D:51:TYR:HD1	1:D:56:THR:HG22	1.66	0.61
1:D:125:VAL:HG21	1:D:159:ILE:CD1	2.31	0.61
1:A:363:VAL:HG22	1:A:440:TYR:HB2	1.82	0.60
1:C:71:HIS:O	1:C:74:VAL:HG23	2.02	0.59
1:D:520:HIS:CG	1:D:532:LEU:HD22	2.38	0.59
1:D:480:LEU:CD1	1:D:480:LEU:O	2.51	0.59
1:C:330:ILE:HG23	1:C:351:LEU:HD22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:480:LEU:O	1:D:480:LEU:HD12	2.03	0.58
1:A:269:SER:OG	1:A:284:ASN:HA	2.03	0.57
1:B:527:THR:O	1:B:527:THR:OG1	2.19	0.57
1:D:269:SER:OG	1:D:285:HIS:ND1	2.34	0.57
1:B:294:LYS:NZ	1:C:319:GLU:OE2	2.38	0.56
1:A:71:HIS:O	1:A:74:VAL:HG23	2.06	0.56
1:A:104:GLN:NE2	3:A:697:HOH:O	2.39	0.56
1:D:554:ALA:HB1	1:D:567:ILE:CD1	2.35	0.56
1:D:488:PHE:HE1	1:D:492:LEU:HD12	1.71	0.55
1:D:36:LEU:HD12	1:D:51:TYR:CD2	2.41	0.55
1:D:214:THR:OG1	1:D:217:GLU:O	2.21	0.55
1:D:260:ALA:HA	1:D:273:ILE:HD13	1.89	0.55
1:B:83:VAL:O	1:B:83:VAL:HG12	2.07	0.54
1:C:272:PHE:HA	1:C:276:GLU:O	2.06	0.54
1:D:137:TYR:HB3	1:D:144:LEU:HD11	1.90	0.54
1:D:50:LEU:CD1	1:D:59:LEU:HD21	2.37	0.54
1:A:427:ALA:HB1	1:A:439:LEU:HD13	1.90	0.54
1:B:262:VAL:HG21	1:B:286:GLY:O	2.06	0.54
1:D:322:LEU:HD22	1:D:326:LEU:HD13	1.90	0.54
1:B:188:ARG:HG3	1:B:190:PHE:CE1	2.43	0.54
1:B:188:ARG:HG3	1:B:190:PHE:CZ	2.43	0.53
1:C:168:GLY:HA3	1:C:170:PHE:CZ	2.43	0.53
1:D:574:PHE:O	1:D:578:GLN:HG2	2.07	0.53
1:D:445:SER:OG	1:D:446:TYR:N	2.39	0.53
1:D:565:VAL:HA	1:D:569:LEU:HB2	1.89	0.53
1:B:51:TYR:HD1	1:B:56:THR:HG22	1.74	0.52
1:D:13:VAL:HG22	1:D:569:LEU:HD21	1.91	0.52
1:B:565:VAL:HA	1:B:569:LEU:HB2	1.91	0.52
1:C:427:ALA:HB1	1:C:439:LEU:HD13	1.92	0.52
1:B:471:VAL:HG13	1:B:477:MET:SD	2.50	0.52
1:D:558:ILE:O	1:D:558:ILE:HG23	2.08	0.52
1:D:125:VAL:HG11	1:D:159:ILE:HD11	1.90	0.51
1:A:168:GLY:HA3	1:A:170:PHE:CZ	2.45	0.51
1:B:84:SER:OG	1:B:87:ALA:HB3	2.11	0.51
1:B:480:LEU:CD1	1:B:480:LEU:O	2.59	0.51
1:B:235:LEU:HD13	1:B:275:GLY:CA	2.41	0.51
1:C:269:SER:OG	1:C:284:ASN:HA	2.11	0.51
1:C:234:GLU:HA	1:C:234:GLU:OE1	2.10	0.50
1:D:159:ILE:CD1	1:D:164:ILE:HG12	2.41	0.50
1:D:71:HIS:O	1:D:72:TYR:C	2.50	0.50
1:D:527:THR:O	1:D:527:THR:OG1	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:ALA:HB1	1:B:567:ILE:CD1	2.42	0.49
1:D:159:ILE:HD13	1:D:164:ILE:HG12	1.93	0.49
1:D:46:VAL:HB	1:D:64:ILE:O	2.13	0.49
1:D:83:VAL:HG22	1:D:83:VAL:O	2.13	0.49
1:A:99:ARG:NE	1:A:102:GLU:OE1	2.43	0.49
1:C:446:TYR:O	1:C:449:TYR:HB3	2.13	0.49
1:A:272:PHE:HA	1:A:276:GLU:O	2.12	0.48
1:C:37:LEU:HD21	1:C:67:VAL:HG21	1.95	0.48
1:D:41:PHE:CD1	1:D:46:VAL:HG22	2.48	0.48
1:D:188:ARG:HG3	1:D:190:PHE:CE1	2.49	0.48
1:D:188:ARG:HG2	1:D:190:PHE:CZ	2.49	0.47
1:A:462:PHE:O	1:A:514:GLU:HG2	2.13	0.47
1:B:327:ARG:CD	3:B:589:HOH:O	2.62	0.47
1:D:27:LEU:HD11	1:D:36:LEU:HD22	1.96	0.47
1:A:529:LEU:HD21	1:A:550:ILE:HD13	1.97	0.47
1:B:574:PHE:O	1:B:578:GLN:HG2	2.16	0.47
1:A:13:VAL:HG21	1:B:13:VAL:HG21	1.96	0.46
1:C:462:PHE:O	1:C:514:GLU:HG2	2.15	0.46
1:B:113:ARG:HB3	1:B:129:ALA:HB3	1.97	0.46
1:B:480:LEU:O	1:B:480:LEU:HD12	2.15	0.46
1:D:262:VAL:HG21	1:D:286:GLY:O	2.16	0.45
1:D:56:THR:HG21	1:D:318:LEU:HD21	1.97	0.45
1:D:536:MET:CE	1:D:550:ILE:HD11	2.46	0.45
1:B:155:PHE:N	1:B:155:PHE:CD1	2.84	0.45
1:D:239:ASP:HB2	1:D:275:GLY:O	2.16	0.45
1:A:301:SER:OG	1:A:304:THR:HG23	2.16	0.45
1:C:472:VAL:HG12	1:C:506:ILE:HB	1.99	0.45
1:D:445:SER:HA	1:D:469:ALA:O	2.16	0.45
1:B:188:ARG:CG	1:B:190:PHE:CZ	2.99	0.45
1:B:125:VAL:HG21	1:B:159:ILE:CD1	2.47	0.45
1:D:50:LEU:HD11	1:D:59:LEU:HD21	1.99	0.45
1:C:529:LEU:HD21	1:C:550:ILE:HD13	1.99	0.45
1:D:188:ARG:CG	1:D:190:PHE:CZ	3.00	0.44
1:B:315:GLU:HG2	3:B:614:HOH:O	2.17	0.44
1:D:561:MET:O	1:D:565:VAL:HG13	2.17	0.44
1:C:547:GLU:HB3	1:D:552:PRO:HD3	2.00	0.44
1:D:488:PHE:CD1	1:D:488:PHE:C	2.91	0.44
1:D:50:LEU:HD12	1:D:59:LEU:HD21	2.00	0.44
1:A:36:LEU:HD11	1:A:291:TRP:CG	2.53	0.44
1:D:27:LEU:HB2	1:D:308:ILE:HD12	2.00	0.44
1:D:223:VAL:HG13	1:D:230:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:GLU:O	1:A:581:ARG:CB	2.66	0.43
1:B:50:LEU:HG	1:B:59:LEU:HD11	1.99	0.43
1:B:431:ARG:NH2	1:B:439:LEU:HD12	2.34	0.43
1:C:301:SER:O	1:C:378:TRP:N	2.52	0.43
1:A:551:ILE:HD13	1:A:567:ILE:HD13	2.01	0.43
1:B:558:ILE:HD11	1:B:564:ALA:HB2	2.01	0.43
1:B:468:GLY:HA2	1:B:519:ILE:O	2.19	0.42
1:D:444:TYR:HA	1:D:468:GLY:O	2.19	0.42
1:C:219:ARG:HB2	3:C:615:HOH:O	2.18	0.42
1:C:337:TRP:CZ3	1:C:347:PRO:HB3	2.54	0.42
1:A:374:ASP:CG	1:A:394:MET:HB3	2.40	0.42
1:B:9:PHE:HB3	1:B:573:PHE:CZ	2.54	0.42
1:B:450:MET:HA	1:B:450:MET:HE2	2.02	0.42
1:A:446:TYR:O	1:A:449:TYR:HB3	2.20	0.42
1:D:219:ARG:NH1	1:D:232:ASP:OD1	2.53	0.42
1:B:476:GLU:OE1	1:B:534:ARG:NH1	2.49	0.42
1:A:301:SER:O	1:A:378:TRP:N	2.52	0.42
1:B:31:VAL:CG2	1:B:50:LEU:HD21	2.50	0.42
1:D:468:GLY:HA2	1:D:519:ILE:O	2.20	0.42
1:B:177:LEU:HD21	1:B:208:VAL:HG11	2.01	0.41
1:B:445:SER:HA	1:B:469:ALA:O	2.20	0.41
1:C:301:SER:OG	1:C:304:THR:HG23	2.20	0.41
1:D:177:LEU:HD22	1:D:223:VAL:HG21	2.01	0.41
1:D:578:GLN:OE1	1:D:581:ARG:NH2	2.53	0.41
1:A:66:SER:OG	2:A:583:GOL:H32	2.20	0.41
1:D:450:MET:HA	1:D:450:MET:CE	2.51	0.41
1:A:234:GLU:HA	1:A:234:GLU:OE1	2.18	0.41
1:B:264:ARG:HD2	3:B:602:HOH:O	2.19	0.41
1:A:5:MET:N	1:A:6:PRO:CD	2.82	0.41
1:B:561:MET:O	1:B:565:VAL:HG13	2.21	0.41
1:D:76:ARG:HA	1:D:97:THR:HG23	2.02	0.41
1:A:476:GLU:HB2	2:A:584:GOL:H2	2.02	0.41
1:A:323:PRO:HG2	1:A:326:LEU:HD12	2.02	0.41
1:A:567:ILE:HD13	1:A:567:ILE:HA	1.88	0.41
1:C:374:ASP:CG	1:C:394:MET:HB3	2.41	0.41
1:A:152:GLY:O	1:A:153:PHE:C	2.57	0.41
1:A:294:LYS:NZ	1:D:276:GLU:OE1	2.49	0.40
1:B:46:VAL:HB	1:B:64:ILE:O	2.22	0.40
1:A:337:TRP:CZ3	1:A:347:PRO:HB3	2.55	0.40
1:A:476:GLU:CB	2:A:584:GOL:H2	2.51	0.40
1:C:381:PHE:CD2	1:C:568:LEU:HD13	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ILE:HD11	1:B:558:ILE:HD11	2.04	0.40
1:D:68:LEU:HD22	1:D:117:GLY:HA3	2.03	0.40
1:A:15:ASP:OD1	1:A:18:ARG:NH1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	575/582 (99%)	561 (98%)	14 (2%)	0	100	100
1	B	570/582 (98%)	549 (96%)	21 (4%)	0	100	100
1	C	574/582 (99%)	558 (97%)	16 (3%)	0	100	100
1	D	574/582 (99%)	546 (95%)	28 (5%)	0	100	100
All	All	2293/2328 (98%)	2214 (97%)	79 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	449/469 (96%)	442 (98%)	7 (2%)	62	84
1	B	426/469 (91%)	412 (97%)	14 (3%)	38	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	447/469 (95%)	439 (98%)	8 (2%)	59	81
1	D	429/469 (92%)	415 (97%)	14 (3%)	38	64
All	All	1751/1876 (93%)	1708 (98%)	43 (2%)	47	73

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASP
1	A	36	LEU
1	A	38	VAL
1	A	304	THR
1	A	352	GLU
1	A	491	GLN
1	A	498	GLU
1	B	34	ASP
1	B	71	HIS
1	B	183	SER
1	B	192	SER
1	B	241	SER
1	B	322	LEU
1	B	334	ARG
1	B	445	SER
1	B	480	LEU
1	B	501	ARG
1	B	510	ASP
1	B	527	THR
1	B	567	ILE
1	B	569	LEU
1	C	32	ASP
1	C	38	VAL
1	C	304	THR
1	C	319	GLU
1	C	352	GLU
1	C	419	GLU
1	C	456	THR
1	C	491	GLN
1	D	34	ASP
1	D	50	LEU
1	D	71	HIS
1	D	183	SER
1	D	241	SER

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Mol	Chain	Res	Type
1	D	326	LEU
1	D	334	ARG
1	D	445	SER
1	D	492	LEU
1	D	510	ASP
1	D	527	THR
1	D	567	ILE
1	D	569	LEU
1	D	581	ARG

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

Mol	Chain	Res	Type
1	A	28	GLN
1	B	28	GLN
1	B	559	ASN
1	C	71	HIS
1	D	28	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 monosaccharides in this entry.

5.6　Ligand geometry ⓘ

4 ligands 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	$\#|Z| > 2$
2	GOL	C	583	-	5,5,5	0.38	0	5,5,5	0.23	0
2	GOL	A	583	-	5,5,5	0.42	0	5,5,5	0.58	0
2	GOL	A	584	-	5,5,5	0.64	0	5,5,5	0.89	0
2	GOL	B	583	-	5,5,5	0.35	0	5,5,5	0.40	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	C	583	-	-	0/4/4/4	-
2	GOL	A	583	-	-	2/4/4/4	-
2	GOL	A	584	-	-	2/4/4/4	-
2	GOL	B	583	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	583	GOL	1	0
2	A	584	GOL	2	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, 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	577/582 (99%)	-0.20	4 (0%)	87	89	32, 42, 55, 64	0
1	B	574/582 (98%)	-0.04	15 (2%)	56	59	30, 46, 70, 84	0
1	C	576/582 (98%)	-0.18	6 (1%)	82	84	31, 42, 56, 67	0
1	D	576/582 (98%)	0.01	22 (3%)	40	43	30, 45, 72, 89	0
All	All	2303/2328 (98%)	-0.10	47 (2%)	65	68	30, 43, 65, 89	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	6	PRO	5.6
1	B	554	ALA	4.9
1	D	141	GLY	4.5
1	D	555	GLY	4.3
1	D	7	VAL	4.3
1	D	341	PHE	4.3
1	D	554	ALA	4.2
1	D	142	GLY	3.9
1	C	6	PRO	3.6
1	B	483	ALA	3.4
1	D	556	HIS	3.3
1	D	132	ASP	3.3
1	A	6	PRO	3.3
1	A	5	MET	3.2
1	D	86	GLY	3.1
1	C	74	VAL	3.0
1	B	482	ASP	2.9
1	D	557	ALA	2.9
1	B	7	VAL	2.7
1	D	54	GLY	2.7
1	D	85	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	580	GLU	2.6
1	B	557	ALA	2.5
1	D	143	GLY	2.5
1	B	193	GLY	2.5
1	A	141	GLY	2.5
1	D	331	ALA	2.4
1	C	244	ARG	2.4
1	D	133	ARG	2.4
1	C	142	GLY	2.2
1	D	484	ALA	2.2
1	B	87	ALA	2.2
1	B	501	ARG	2.2
1	B	74	VAL	2.2
1	B	86	GLY	2.2
1	B	481	SER	2.2
1	D	480	LEU	2.1
1	B	85	LYS	2.1
1	C	293	GLY	2.1
1	D	193	GLY	2.1
1	C	141	GLY	2.1
1	B	580	GLU	2.1
1	B	523	ASN	2.1
1	B	131	GLU	2.1
1	D	131	GLU	2.0
1	D	497	ARG	2.0
1	D	581	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	A	583	6/6	0.74	0.14	56,58,59,60	0
2	GOL	B	583	6/6	0.74	0.27	54,58,58,59	0
2	GOL	A	584	6/6	0.83	0.29	36,44,46,47	0
2	GOL	C	583	6/6	0.87	0.26	54,57,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.