

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	4AG5
Title	:	Structure of VirB4 of Thermoanaerobacter pseudethanolicus
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Deposited on	:	2012-01-24
Resolution	:	2.45 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 following versions of software and data (see references (1)) 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	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.45 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	А	392	% •	8%		24%	• 5%	
1	В	392	66	9%		27%	• 5%	
1	С	392	4%	20%	•	32%		
1	D	392	14%	27%	•	31%		



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10083 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 TYPE IV SECRETORY PATHWAY VIRB4 COMPONENTS-LIKE PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	374	Total	С	Ν	Ο	S	0	0	0
	Л	574	2941	1875	502	555	9	0	0	
1	В	374	Total	С	Ν	Ο	S	0	0	0
	D	374	2935	1868	502	556	9	0	0	
1	C	26.8	Total	С	Ν	Ο	S	0	0	0
	U	208	1994	1280	331	378	5	0	0	0
1	1 D	270	Total	С	Ν	Ο	S	0	0	0
			1972	1265	327	377	3	0	0	0

• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total Mg 1 1	0	0
2	А	1	Total Mg 1 1	0	0
2	С	1	Total Mg 1 1	0	0

• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0

• Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	Λ	1	Total	С	Ν	Ο	Р	0	0
4	A	1	27	10	5	10	2	0	0
4	р	1	Total	С	Ν	Ο	Р	0	0
'1	D		27	10	5	10	2	U	U

• Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	А	1	Total 5	O 4	S 1	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	70	Total O 70 70	0	0
6	В	65	Total O 65 65	0	0
6	С	12	Total O 12 12	0	0
6	D	14	Total O 14 14	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: TYPE IV SECRETORY PATHWAY VIRB4 COMPONENTS-LIKE PROTEIN











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants	108.08Å 110.80 Å 156.43 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	54.04 - 2.45	Depositor
Resolution (A)	54.04 - 2.45	EDS
% Data completeness	95.8 (54.04-2.45)	Depositor
(in resolution range)	95.4(54.04-2.45)	EDS
R _{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.98 (at 2.45 \text{\AA})$	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
D D	0.233 , 0.288	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.232 , 0.287	DCC
R_{free} test set	3496 reflections $(5.04%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	46.2	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33 , 72.3	EDS
L-test for twinning ²	$< L > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10083	wwPDB-VP
Average B, all atoms $(Å^2)$	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 9.06% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: GOL, MG, SO4, ADP

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).

Mal	Chain	Bond	lengths	Bond angles		
10101	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.41	0/2998	0.56	0/4068	
1	В	0.37	0/2992	0.56	0/4061	
1	С	0.35	0/2036	0.55	0/2786	
1	D	0.39	0/2005	0.61	3/2739~(0.1%)	
All	All	0.38	0/10031	0.57	3/13654~(0.0%)	

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	D	287	VAL	N-CA-CB	-7.53	94.94	111.50
1	D	287	VAL	N-CA-C	6.51	128.56	111.00
1	D	286	GLY	N-CA-C	-5.30	99.86	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2941	0	2895	77	0
1	В	2935	0	2884	81	0
1	С	1994	0	1805	54	0
1	D	1972	0	1780	104	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	А	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
3	А	12	0	16	3	0
3	В	6	0	8	0	0
4	А	27	0	12	0	0
4	В	27	0	12	3	0
5	А	5	0	0	0	0
6	А	70	0	0	3	0
6	В	65	0	0	2	0
6	С	12	0	0	1	0
6	D	14	0	0	1	0
All	All	10083	0	9412	312	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 16.

All (312) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:398:ARG:HH11	1:D:398:ARG:HG2	1.20	1.06
1:B:569:VAL:HG22	1:B:574:ARG:HG2	1.37	1.03
1:D:503:ILE:HG22	1:D:505:ILE:HD11	1.44	0.97
1:D:372:ASN:O	1:D:418:PRO:HB3	1.75	0.85
1:D:270:ILE:HD13	1:D:277:TYR:CD2	2.12	0.84
1:D:272:ASP:OD2	1:D:277:TYR:HD1	1.61	0.82
1:B:271:ILE:HD12	1:B:470:VAL:HG12	1.62	0.81
1:A:444:ARG:HG2	1:A:475:MET:O	1.81	0.81
1:D:449:ASN:HD22	1:D:449:ASN:C	1.86	0.79
1:C:341:THR:HG22	1:C:344:GLU:H	1.47	0.78
1:D:398:ARG:CG	1:D:398:ARG:HH11	1.93	0.78
1:D:270:ILE:CD1	1:D:277:TYR:CD2	2.68	0.77
1:C:338:ARG:HH12	1:C:478:ASP:CG	1.87	0.76
1:B:214:VAL:HG12	1:B:223:LEU:HD21	1.68	0.75
1:A:241:THR:HG23	1:A:528:PRO:HG2	1.68	0.75
1:A:218:ASP:HB2	1:A:222:GLY:H	1.52	0.75
1:D:391:GLU:HG3	1:D:392:ASN:HD22	1.53	0.74
1:B:509:VAL:HG13	1:B:540:ASP:CG	2.08	0.73
1:D:503:ILE:HG22	1:D:505:ILE:CD1	2.19	0.73
1:C:290:ASN:O	1:C:296:GLY:HA3	1.89	0.72
1:D:270:ILE:HD13	1:D:277:TYR:CE2	2.25	0.71



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:299:ASN:N	1:D:419:THR:HG1	1.88	0.71
1:C:382:TYR:O	1:C:386:VAL:HG23	1.92	0.70
1:C:287:VAL:HG12	1:C:425:SER:HB3	1.73	0.69
1:C:257:LEU:O	1:C:261:GLU:HG2	1.92	0.69
1:D:459:GLU:OE2	6:D:2011:HOH:O	2.09	0.69
1:C:305:LEU:HD23	1:C:459:GLU:HG2	1.75	0.69
1:A:555:HIS:O	1:A:559:VAL:HG23	1.93	0.69
1:A:573:GLN:HG3	3:A:1590:GOL:H11	1.77	0.67
1:D:323:ALA:HB2	1:D:363:TRP:HZ3	1.59	0.66
1:D:341:THR:O	1:D:345:LYS:HG3	1.95	0.66
1:C:361:ILE:HG13	1:C:361:ILE:O	1.96	0.65
4:B:1589:ADP:H4'	1:D:236:THR:HG21	1.78	0.65
1:D:329:LEU:O	1:D:333:PHE:HD2	1.78	0.65
1:D:503:ILE:CG2	1:D:505:ILE:HD11	2.22	0.65
1:B:339:ASP:CG	1:B:398:ARG:HH22	2.00	0.65
1:C:292:THR:HG21	1:C:434:ASP:HB2	1.78	0.65
1:D:398:ARG:NH1	1:D:398:ARG:HG2	2.00	0.64
1:D:447:TYR:OH	1:D:470:VAL:HG13	1.98	0.63
1:D:470:VAL:HG12	1:D:473:ALA:HB2	1.80	0.63
1:B:240:TRP:HB2	1:B:503:ILE:HG12	1.80	0.63
1:A:531:LYS:HB2	1:A:569:VAL:HB	1.79	0.63
1:D:467:VAL:HA	1:D:501:SER:O	1.99	0.63
1:D:455:TRP:CE3	1:D:491:THR:HG23	2.33	0.62
1:B:297:LYS:O	1:B:419:THR:HA	2.00	0.62
1:A:344:GLU:OE2	1:A:398:ARG:NH1	2.32	0.62
1:B:422:GLU:H	1:B:422:GLU:CD	2.02	0.62
1:B:321:PRO:HD2	6:B:2033:HOH:O	1.99	0.62
1:D:321:PRO:O	1:D:324:LEU:HD12	2.00	0.62
1:B:291:CYS:HA	1:B:296:GLY:O	1.98	0.61
1:D:322:LEU:O	1:D:326:ILE:HG12	2.00	0.61
1:A:218:ASP:HB3	1:A:220:ASP:H	1.64	0.61
1:A:426:ASP:HB3	1:A:463:ARG:HH22	1.66	0.61
1:B:355:VAL:HG21	1:B:381:LEU:HA	1.81	0.61
1:C:527:ASN:N	1:C:528:PRO:HD2	2.15	0.61
1:D:327:GLN:HA	1:D:330:ARG:HG2	1.80	0.61
1:D:337:LEU:HB3	1:D:340:LEU:HD13	1.83	0.60
1:C:252:PHE:O	1:C:255:LYS:HB2	2.01	0.60
1:D:441:GLN:HG2	1:D:442:VAL:N	2.16	0.60
1:B:516:GLU:N	1:B:516:GLU:OE1	2.28	0.60
1:C:336:TYR:CD2	1:C:337:LEU:HD13	2.37	0.60
1:D:270:ILE:HG12	1:D:469:VAL:HB	1.84	0.60



	lous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:356:TYR:CD1	1:D:361:ILE:HD11	2.37	0.60
1:D:370:VAL:O	1:D:370:VAL:HG22	2.02	0.59
1:A:218:ASP:HB2	1:A:222:GLY:N	2.16	0.59
1:A:344:GLU:CD	1:A:398:ARG:HH12	2.06	0.59
1:C:461:ASP:O	1:C:463:ARG:N	2.32	0.59
1:A:305:LEU:HD23	1:A:367:PRO:HB2	1.84	0.59
1:B:382:TYR:O	1:B:386:VAL:HG23	2.03	0.58
1:B:241:THR:HG22	1:B:243:LEU:HG	1.84	0.58
1:B:538:GLU:CD	1:B:538:GLU:H	2.07	0.58
1:B:436:GLN:HA	1:B:443:LYS:NZ	2.19	0.57
1:D:324:LEU:HD12	1:D:325:HIS:H	1.69	0.57
1:C:385:CYS:O	1:C:389:ALA:HB2	2.04	0.57
1:A:384:TYR:CZ	1:A:388:LYS:NZ	2.68	0.57
1:D:323:ALA:HB2	1:D:363:TRP:CZ3	2.39	0.57
1:B:585:GLU:C	1:B:587:GLN:H	2.07	0.57
1:B:306:ARG:HB2	1:B:307:PRO:HD2	1.87	0.57
1:D:391:GLU:HG3	1:D:392:ASN:ND2	2.17	0.57
1:A:379:LYS:O	1:A:383:GLU:HG3	2.05	0.56
1:B:336:TYR:CD2	1:B:337:LEU:HD13	2.40	0.56
1:D:361:ILE:O	1:D:361:ILE:HG13	2.04	0.56
1:D:327:GLN:O	1:D:330:ARG:HG2	2.06	0.56
1:A:530:TYR:HA	1:A:569:VAL:O	2.05	0.56
1:B:337:LEU:HB3	1:B:340:LEU:HD13	1.86	0.56
1:A:241:THR:CG2	1:A:528:PRO:HG2	2.35	0.55
1:B:234:ASP:OD1	1:B:571:GLY:HA3	2.06	0.55
1:C:421:VAL:HA	6:C:2001:HOH:O	2.05	0.55
1:C:308:VAL:HG11	1:C:319:GLN:HE22	1.71	0.55
1:D:449:ASN:C	1:D:449:ASN:ND2	2.55	0.55
1:D:287:VAL:HG13	1:D:287:VAL:O	2.06	0.55
1:C:330:ARG:HD2	1:C:349:GLU:OE2	2.06	0.55
1:D:325:HIS:O	1:D:329:LEU:HD13	2.07	0.55
1:A:512:PHE:O	1:A:517:VAL:HG23	2.06	0.55
1:A:384:TYR:CE2	1:A:388:LYS:NZ	2.74	0.55
1:D:405:ARG:HA	1:D:409:GLY:HA3	1.88	0.55
1:A:573:GLN:CG	3:A:1590:GOL:H11	2.38	0.54
1:A:233:GLY:HA3	6:A:2007:HOH:O	2.05	0.54
1:A:461:ASP:O	1:A:463:ARG:HG2	2.07	0.54
1:A:355:VAL:HG21	1:A:381:LEU:HA	1.89	0.54
1:D:321:PRO:HA	1:D:324:LEU:HD11	1.90	0.54
1:A:224:VAL:HG11	1:A:577:ILE:HG13	1.89	0.54
1:D:441:GLN:HG2	1:D:442:VAL:H	1.72	0.54



	to as pagen	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:526:ASP:HA	1:B:531:LYS:HE3	1.90	0.54
1:D:275:ARG:HE	1:D:431:ASP:CG	2.11	0.53
1:A:256:MET:O	1:A:260:ARG:HG3	2.08	0.53
1:A:569:VAL:HG22	1:A:574:ARG:HD3	1.90	0.53
1:B:461:ASP:OD1	1:B:461:ASP:O	2.27	0.53
1:D:270:ILE:CD1	1:D:277:TYR:CE2	2.90	0.53
1:D:446:GLN:OE1	1:D:446:GLN:HA	2.09	0.53
1:A:257:LEU:O	1:A:261:GLU:HG2	2.09	0.53
1:D:243:LEU:O	1:D:244:ALA:HB2	2.09	0.53
1:D:388:LYS:HB3	1:D:396:TYR:CD2	2.44	0.53
1:B:322:LEU:O	1:B:326:ILE:HG12	2.08	0.53
1:B:277:TYR:HD1	1:B:280:MET:CE	2.22	0.52
1:B:236:THR:O	1:B:496:ARG:HD3	2.09	0.52
1:C:379:LYS:HA	1:C:407:ALA:HB1	1.91	0.52
1:B:274:GLU:HB2	1:B:276:GLU:HG2	1.92	0.52
1:A:235:ARG:HB3	6:A:2005:HOH:O	2.09	0.52
1:B:422:GLU:N	1:B:422:GLU:CD	2.62	0.52
1:A:240:TRP:HB2	1:A:503:ILE:HG12	1.92	0.52
1:B:436:GLN:HA	1:B:443:LYS:HZ1	1.72	0.52
1:D:299:ASN:HB2	1:D:417:GLY:O	2.10	0.52
1:D:398:ARG:HH12	1:D:402:LEU:HD22	1.75	0.52
1:B:446:GLN:HA	1:B:446:GLN:OE1	2.10	0.51
1:C:370:VAL:HG22	1:C:375:TRP:CE2	2.45	0.51
1:C:527:ASN:N	1:C:528:PRO:CD	2.73	0.51
1:A:470:VAL:HG23	1:A:470:VAL:O	2.09	0.51
1:B:527:ASN:N	1:B:528:PRO:CD	2.73	0.51
1:A:213:ILE:HD11	1:A:257:LEU:HD12	1.92	0.51
1:D:355:VAL:HG21	1:D:381:LEU:HA	1.93	0.51
1:A:267:ARG:CZ	1:A:463:ARG:HG3	2.40	0.51
1:D:494:ARG:O	1:D:497:LYS:N	2.43	0.51
1:B:391:GLU:HG3	1:B:392:ASN:ND2	2.26	0.51
1:D:470:VAL:HG12	1:D:470:VAL:O	2.10	0.51
1:D:288:TRP:CD1	1:D:429:VAL:HB	2.45	0.51
1:A:347:ALA:HB1	1:A:396:TYR:CZ	2.47	0.50
1:A:513:LEU:HD23	1:A:543:ALA:HB1	1.94	0.50
1:B:254:ALA:O	1:B:258:LEU:HG	2.12	0.50
1:D:443:LYS:HD2	1:D:444:ARG:N	2.26	0.50
1:B:426:ASP:CG	1:B:463:ARG:HH22	2.14	0.50
1:A:305:LEU:CD2	1:A:367:PRO:HB2	2.41	0.50
1:A:573:GLN:CD	3:A:1590:GOL:H11	2.32	0.50
1:A:301:LEU:HD23	1:A:301:LEU:N	2.27	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:322:LEU:O	1:A:326:ILE:HG12	2.12	0.50
1:B:290:ASN:O	1:B:296:GLY:HA3	2.12	0.49
1:B:433:HIS:C	1:B:435:LEU:H	2.15	0.49
1:D:325:HIS:HA	1:D:328:THR:HG23	1.95	0.49
1:C:521:GLY:O	1:C:525:LEU:HG	2.11	0.49
1:D:511:ASP:O	1:D:517:VAL:HG21	2.12	0.49
1:A:398:ARG:HB3	1:A:398:ARG:HH11	1.78	0.49
1:B:304:ARG:HB2	1:B:456:ASN:CG	2.31	0.49
1:D:275:ARG:HG2	1:D:431:ASP:OD2	2.12	0.49
1:A:241:THR:HG21	1:A:525:LEU:HA	1.94	0.49
1:B:413:TYR:OH	1:B:435:LEU:HD21	2.13	0.49
1:D:303:VAL:HA	1:D:325:HIS:CG	2.48	0.49
1:B:347:ALA:HB1	1:B:396:TYR:CZ	2.47	0.49
1:A:302:GLN:O	1:A:304:ARG:HD3	2.13	0.49
1:A:214:VAL:O	1:A:260:ARG:NH1	2.45	0.49
1:B:256:MET:HB3	1:B:260:ARG:HH11	1.78	0.49
1:A:262:TYR:HD2	1:A:263:MET:HE2	1.78	0.49
1:C:308:VAL:HG11	1:C:319:GLN:NE2	2.28	0.49
1:C:461:ASP:OD1	1:C:461:ASP:O	2.30	0.49
1:D:477:VAL:HA	1:D:485:ILE:HD11	1.95	0.49
1:A:433:HIS:O	1:A:436:GLN:HG2	2.14	0.48
1:A:444:ARG:HD2	1:A:478:ASP:HB2	1.95	0.48
1:A:518:GLN:NE2	1:B:542:GLU:HG3	2.27	0.48
1:C:308:VAL:HG22	1:C:309:GLU:N	2.27	0.48
1:C:391:GLU:CD	1:C:392:ASN:HD22	2.16	0.48
1:C:344:GLU:OE1	1:C:398:ARG:NH1	2.46	0.48
1:B:585:GLU:C	1:B:587:GLN:N	2.67	0.48
1:C:455:TRP:CZ3	1:C:458:LEU:HD23	2.47	0.48
1:B:255:LYS:HG2	1:B:280:MET:HE2	1.95	0.48
1:D:274:GLU:HA	1:D:433:HIS:ND1	2.28	0.48
1:A:299:ASN:C	1:A:299:ASN:OD1	2.52	0.48
1:B:477:VAL:HA	1:B:485:ILE:HD11	1.95	0.48
1:B:398:ARG:HA	1:B:401:VAL:HG12	1.96	0.47
1:D:251:SER:O	1:D:255:LYS:HG2	2.13	0.47
1:A:213:ILE:CD1	1:A:257:LEU:HD12	2.44	0.47
1:B:218:ASP:HB3	1:B:220:ASP:H	1.79	0.47
1:B:444:ARG:HD3	1:B:475:MET:O	2.14	0.47
1:C:304:ARG:HB2	1:C:456:ASN:CG	2.35	0.47
1:D:514:ALA:HB3	1:D:517:VAL:HG22	1.97	0.47
1:B:530:TYR:HA	1:B:569:VAL:O	2.15	0.47
1:B:327:GLN:O	1:B:330:ARG:HB2	2.15	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:478:ASP:OD1	1:B:478:ASP:C	2.52	0.47
1:B:267:ARG:NH1	1:B:463:ARG:HD3	2.29	0.47
1:D:476:LEU:HD13	1:D:485:ILE:HD13	1.97	0.47
1:D:290:ASN:HA	1:D:431:ASP:HB3	1.97	0.47
1:D:374:LYS:HG3	1:D:374:LYS:O	2.14	0.47
1:B:333:PHE:O	1:B:337:LEU:HB2	2.15	0.47
1:D:492:SER:HB2	1:D:502:LEU:HD22	1.97	0.47
1:A:263:MET:CE	1:A:263:MET:HA	2.45	0.46
1:D:443:LYS:C	1:D:443:LYS:HD2	2.36	0.46
1:C:446:GLN:OE1	1:C:446:GLN:HA	2.14	0.46
1:D:444:ARG:HG3	1:D:475:MET:O	2.15	0.46
1:A:534:LEU:O	1:A:536:GLN:NE2	2.49	0.46
1:B:243:LEU:O	1:B:244:ALA:HB2	2.15	0.46
1:B:523:ALA:O	1:B:527:ASN:HB2	2.15	0.46
1:B:582:ALA:O	1:B:585:GLU:HB2	2.15	0.46
1:C:403:LEU:HD12	1:C:403:LEU:HA	1.79	0.46
1:A:306:ARG:C	1:A:459:GLU:OE1	2.54	0.46
1:A:459:GLU:HG2	1:A:498:TYR:OH	2.15	0.46
1:D:244:ALA:O	1:D:507:GLN:HA	2.16	0.46
1:C:491:THR:HG22	1:C:502:LEU:HD22	1.98	0.46
1:D:470:VAL:CG1	1:D:473:ALA:HB2	2.44	0.46
1:D:495:ILE:HD13	1:D:501:SER:C	2.37	0.46
1:B:538:GLU:CD	1:B:538:GLU:N	2.69	0.45
1:D:248:ALA:O	1:D:534:LEU:HD23	2.16	0.45
1:B:219:ARG:HG3	1:B:220:ASP:OD1	2.16	0.45
1:D:262:TYR:C	1:D:264:GLN:N	2.69	0.45
1:A:361:ILE:HD13	1:A:375:TRP:HZ3	1.81	0.45
1:A:272:ASP:OD1	1:A:275:ARG:N	2.49	0.45
1:D:324:LEU:HD12	1:D:325:HIS:N	2.31	0.45
1:D:331:THR:O	1:D:332:PHE:C	2.52	0.45
1:A:482:PRO:HB3	1:A:517:VAL:HG12	1.99	0.45
1:B:436:GLN:HA	1:B:436:GLN:OE1	2.17	0.45
1:A:258:LEU:HD11	1:A:469:VAL:HG21	1.98	0.45
1:C:338:ARG:NH1	1:C:478:ASP:OD2	2.48	0.45
1:C:488:LEU:O	1:C:491:THR:HB	2.17	0.45
1:D:481:THR:C	1:D:483:GLN:H	2.19	0.45
1:A:304:ARG:HG2	1:A:325:HIS:CE1	2.52	0.45
1:A:337:LEU:HD22	1:A:402:LEU:HB3	1.99	0.45
1:C:306:ARG:HB2	1:C:307:PRO:HD2	1.99	0.45
1:C:263:MET:O	1:C:264:GLN:C	2.55	0.44
1:C:322:LEU:HD11	1:C:356:TYR:CD2	2.52	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:213:ILE:O	1:A:225:LEU:HD23	2.17	0.44
1:D:536:GLN:NE2	1:D:544:ILE:HD13	2.33	0.44
1:B:256:MET:HB3	1:B:260:ARG:NH1	2.33	0.44
1:A:327:GLN:O	1:A:330:ARG:HB2	2.17	0.44
1:C:308:VAL:HG21	1:C:319:GLN:OE1	2.17	0.44
1:D:329:LEU:HD23	1:D:352:LEU:HD13	1.99	0.44
1:B:320:SER:HB3	1:B:323:ALA:HB3	1.99	0.44
1:B:440:ASP:O	1:B:443:LYS:HB2	2.16	0.44
1:B:343:THR:HG23	1:C:320:SER:HB3	1.99	0.44
1:D:382:TYR:O	1:D:386:VAL:HG23	2.17	0.44
1:B:252:PHE:CE1	4:B:1589:ADP:C6	3.06	0.44
1:D:271:ILE:HD11	1:D:451:LEU:HA	1.99	0.44
1:D:533:LEU:HD22	1:D:544:ILE:HD12	1.99	0.44
1:A:459:GLU:HG2	1:A:498:TYR:CE2	2.52	0.43
1:B:255:LYS:HG2	1:B:280:MET:CE	2.47	0.43
1:C:302:GLN:HG3	1:C:375:TRP:CD1	2.53	0.43
1:B:477:VAL:HG11	1:B:511:ASP:O	2.17	0.43
1:B:522:GLN:HG3	1:B:547:LEU:HD11	2.00	0.43
1:C:300:PRO:O	1:C:329:LEU:HD21	2.19	0.43
1:A:253:THR:HG21	1:A:532:LEU:CD1	2.49	0.43
1:B:297:LYS:HE2	1:B:413:TYR:O	2.18	0.43
1:D:398:ARG:NH1	1:D:398:ARG:CG	2.62	0.43
1:B:477:VAL:HG22	1:B:485:ILE:CD1	2.49	0.43
1:D:495:ILE:CG2	1:D:496:ARG:N	2.81	0.43
1:A:532:LEU:HD23	1:A:532:LEU:HA	1.93	0.43
1:D:262:TYR:O	1:D:264:GLN:N	2.52	0.43
1:A:442:VAL:O	1:A:443:LYS:C	2.58	0.42
1:A:458:LEU:HD22	1:A:495:ILE:HG13	2.00	0.42
1:A:324:LEU:HA	1:A:324:LEU:HD12	1.86	0.42
1:D:262:TYR:C	1:D:264:GLN:H	2.21	0.42
4:B:1589:ADP:H4'	1:D:236:THR:CG2	2.48	0.42
1:B:218:ASP:HB2	1:B:222:GLY:N	2.34	0.42
1:C:300:PRO:CD	1:C:415:TRP:HB3	2.50	0.42
1:C:293:GLY:HA2	1:C:413:TYR:O	2.20	0.42
1:D:382:TYR:HE1	1:D:400:SER:O	2.01	0.42
1:B:294:GLY:HA2	1:B:297:LYS:HE3	2.02	0.42
1:D:303:VAL:HB	1:D:375:TRP:CH2	2.55	0.42
1:C:306:ARG:HB2	1:C:307:PRO:CD	2.50	0.42
1:A:413:TYR:CE2	1:A:414:LEU:CD2	3.03	0.42
1:C:278:LYS:O	1:C:279:GLU:C	2.58	0.42
1:D:327:GLN:O	1:D:328:THR:C	2.57	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:531:LYS:HD3	1:A:548:MET:CE	2.50	0.41
1:B:567:LEU:CD2	1:B:574:ARG:HD2	2.50	0.41
1:A:303:VAL:HG13	1:A:325:HIS:HB2	2.02	0.41
1:C:287:VAL:CG1	1:C:425:SER:HB3	2.45	0.41
1:B:337:LEU:HD12	1:B:337:LEU:HA	1.74	0.41
1:A:335:LEU:O	1:A:441:GLN:HB2	2.20	0.41
1:C:335:LEU:HA	1:C:335:LEU:HD23	1.85	0.41
1:C:495:ILE:HG12	1:C:500:GLY:HA3	2.03	0.41
1:A:471:ASP:CG	6:A:2017:HOH:O	2.59	0.41
1:B:477:VAL:HG22	1:B:485:ILE:HD11	2.01	0.41
1:B:495:ILE:HG12	1:B:500:GLY:HA3	2.02	0.41
1:C:307:PRO:HB2	1:C:490:ASP:HB3	2.01	0.41
1:D:281:CYS:SG	1:D:288:TRP:HB2	2.60	0.41
1:D:275:ARG:NH2	1:D:434:ASP:OD1	2.52	0.41
1:A:273:PRO:HG2	1:A:472:GLU:HB2	2.02	0.41
1:B:214:VAL:HG12	1:B:223:LEU:CD2	2.46	0.41
1:B:509:VAL:HG13	1:B:540:ASP:CB	2.49	0.41
1:D:270:ILE:HG12	1:D:469:VAL:CG1	2.50	0.41
1:D:474:TRP:HA	1:D:477:VAL:HG23	2.03	0.41
1:A:243:LEU:O	1:A:244:ALA:HB2	2.20	0.41
1:A:303:VAL:HG13	1:A:325:HIS:CB	2.51	0.41
1:D:270:ILE:HD13	1:D:277:TYR:CG	2.54	0.41
1:D:303:VAL:HG13	1:D:325:HIS:HB2	2.03	0.41
1:A:364:ASP:CG	1:D:394:GLU:HB2	2.41	0.41
1:C:355:VAL:HG21	1:C:381:LEU:HA	2.03	0.41
1:D:287:VAL:O	1:D:287:VAL:CG1	2.69	0.41
1:D:341:THR:OG1	1:D:344:GLU:HG3	2.21	0.41
1:D:300:PRO:CD	1:D:415:TRP:HB3	2.51	0.41
1:B:496:ARG:NH2	6:B:2056:HOH:O	2.54	0.41
1:B:518:GLN:HE21	1:B:518:GLN:HB2	1.70	0.41
1:C:482:PRO:HB3	1:C:517:VAL:HG12	2.03	0.41
1:A:318:PHE:CZ	1:D:394:GLU:HB3	2.55	0.41
1:A:462:ARG:H	1:A:462:ARG:HG2	1.51	0.40
1:B:302:GLN:O	1:B:304:ARG:HD3	2.21	0.40
1:C:299:ASN:HB2	1:C:417:GLY:O	2.20	0.40
1:C:405:ARG:HA	1:C:409:GLY:HA3	2.02	0.40
1:C:413:TYR:OH	1:C:435:LEU:HD21	2.21	0.40
1:C:476:LEU:HD12	1:C:476:LEU:HA	1.83	0.40
1:D:262:TYR:CD2	1:D:262:TYR:C	2.94	0.40
1:B:214:VAL:CG1	1:B:223:LEU:HD21	2.42	0.40
1:D:231:ARG:HG3	1:D:232:GLY:N	2.37	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:481:THR:O	1:D:481:THR:HG22	2.21	0.40
1:A:297:LYS:NZ	1:A:297:LYS:HB2	2.36	0.40
1:D:270:ILE:O	1:D:270:ILE:HG22	2.21	0.40
1:B:244:ALA:HB2	1:B:534:LEU: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	Perce	entiles
1	А	370/392~(94%)	$351 \ (95\%)$	17 (5%)	2 (0%)	29	34
1	В	370/392~(94%)	346~(94%)	23~(6%)	1 (0%)	41	49
1	С	258/392~(66%)	228~(88%)	28 (11%)	2 (1%)	19	22
1	D	252/392~(64%)	239~(95%)	12 (5%)	1 (0%)	34	41
All	All	1250/1568~(80%)	1164 (93%)	80 (6%)	6 (0%)	29	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	462	ARG
1	В	293	GLY
1	С	462	ARG
1	D	230	LYS
1	А	423	ALA
1	С	416	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	А	304/330~(92%)	285~(94%)	19 (6%)	18	22
1	В	304/330~(92%)	283~(93%)	21 (7%)	15	18
1	С	186/330~(56%)	169~(91%)	17 (9%)	9	10
1	D	179/330~(54%)	158 (88%)	21 (12%)	5	4
All	All	973/1320~(74%)	895~(92%)	78 (8%)	12	14

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

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	217	LYS
1	А	224	VAL
1	А	225	LEU
1	А	304	ARG
1	А	324	LEU
1	А	341	THR
1	А	361	ILE
1	А	403	LEU
1	А	429	VAL
1	А	458	LEU
1	А	462	ARG
1	А	463	ARG
1	А	480	GLN
1	А	488	LEU
1	А	506	SER
1	А	513	LEU
1	А	532	LEU
1	А	534	LEU
1	А	577	ILE
1	В	224	VAL
1	В	225	LEU
1	В	304	ARG
1	В	337	LEU
1	В	340	LEU
1	В	362	THR
1	В	370	VAL
1	В	403	LEU
1	В	422	GLU



Mol	Chain	Res	Type
1	В	444	ARG
1	В	476	LEU
1	В	488	LEU
1	В	489	ARG
1	В	493	LYS
1	В	506	SER
1	В	509	VAL
1	В	513	LEU
1	В	518	GLN
1	В	532	LEU
1	В	534	LEU
1	В	538	GLU
1	С	253	THR
1	С	304	ARG
1	С	305	LEU
1	C	308	VAL
1	С	337	LEU
1	С	341	THR
1	С	361	ILE
1	С	362	THR
1	С	370	VAL
1	С	378	VAL
1	С	391	GLU
1	С	403	LEU
1	С	421	VAL
1	С	447	TYR
1	С	470	VAL
1	С	525	LEU
1	С	529	THR
1	D	236	THR
1	D	281	CYS
1	D	284	LEU
1	D	301	LEU
1	D	324	LEU
1	D	328	THR
1	D	334	SER
1	D	337	LEU
1	D	340	LEU
1	D	361	ILE
1	D	370	VAL
1	D	374	LYS
1	D	378	VAL



Contr	Continuea from previous page									
Mol	Chain	\mathbf{Res}	Type							
1	D	398	ARG							
1	D	443	LYS							
1	D	447	TYR							
1	D	449	ASN							
1	D	452	SER							
1	D	467	VAL							
1	D	488	LEU							
1	D	516	GLU							

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

Mol	Chain	Res	Type
1	А	208	ASN
1	А	290	ASN
1	А	319	GLN
1	А	518	GLN
1	А	555	HIS
1	В	518	GLN
1	В	527	ASN
1	D	239	ASN
1	D	480	GLN
1	D	536	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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 Tuno Chair		Chain	Dec	Tink	Bond lengths			Bond angles		
	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	А	1592	-	4,4,4	0.14	0	$6,\!6,\!6$	0.07	0
3	GOL	А	1590	-	5, 5, 5	0.37	0	$5,\!5,\!5$	0.32	0
3	GOL	А	1593	-	5, 5, 5	0.35	0	$5,\!5,\!5$	0.25	0
4	ADP	В	1589	2	24, 29, 29	1.05	3 (12%)	$29,\!45,\!45$	1.36	3 (10%)
3	GOL	В	1590	-	5, 5, 5	0.39	0	$5,\!5,\!5$	0.27	0
4	ADP	А	1591	2	24, 29, 29	1.00	2 (8%)	29,45,45	1.36	3 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	А	1593	-	-	4/4/4/4	-
4	ADP	В	1589	2	-	2/12/32/32	0/3/3/3
3	GOL	В	1590	-	-	2/4/4/4	-
4	ADP	А	1591	2	-	2/12/32/32	0/3/3/3
3	GOL	А	1590	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
4	В	1589	ADP	C5-C4	2.72	1.48	1.40
4	А	1591	ADP	C5-C4	2.40	1.47	1.40
4	А	1591	ADP	O4'-C1'	2.23	1.44	1.41
4	В	1589	ADP	C2-N3	2.19	1.35	1.32
4	В	1589	ADP	O4'-C1'	2.02	1.43	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	1591	ADP	N3-C2-N1	-3.07	123.88	128.68
4	А	1591	ADP	C4-C5-N7	-2.93	106.35	109.40



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$		
4	В	1589	ADP	N3-C2-N1	-2.83	124.25	128.68		
4	В	1589	ADP	C3'-C2'-C1'	2.59	104.88	100.98		
4	В	1589	ADP	C4-C5-N7	-2.32	106.99	109.40		
4	А	1591	ADP	C3'-C2'-C1'	2.31	104.46	100.98		

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
4	В	1589	ADP	PA-O3A-PB-O2B
3	А	1590	GOL	C1-C2-C3-O3
3	А	1593	GOL	O1-C1-C2-C3
3	В	1590	GOL	C1-C2-C3-O3
3	В	1590	GOL	O2-C2-C3-O3
4	А	1591	ADP	PA-O3A-PB-O2B
3	А	1590	GOL	O2-C2-C3-O3
3	А	1593	GOL	O1-C1-C2-O2
3	А	1593	GOL	C1-C2-C3-O3
3	А	1593	GOL	O2-C2-C3-O3
4	В	1589	ADP	PA-O3A-PB-O1B
4	А	1591	ADP	PA-O3A-PB-O3B

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	1590	GOL	3	0
4	В	1589	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	$Q{<}0.9$
1	А	374/392~(95%)	-0.03	3 (0%) 86 86	23, 47, 77, 97	0
1	В	374/392~(95%)	-0.01	0 100 100	31, 52, 87, 132	0
1	С	268/392~(68%)	0.31	16 (5%) 21 18	39, 84, 131, 158	0
1	D	270/392~(68%)	0.88	55~(20%) 1 0	57, 86, 118, 181	0
All	All	1286/1568~(82%)	0.24	74 (5%) 23 20	23, 62, 113, 181	0

All (74) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	D	430	PHE	5.8
1	D	512	PHE	5.4
1	D	458	LEU	5.3
1	D	515	PRO	5.0
1	D	485	ILE	4.7
1	D	504	VAL	4.7
1	D	513	LEU	4.4
1	D	271	ILE	4.0
1	С	282	ARG	4.0
1	D	524	LEU	3.9
1	D	489	ARG	3.7
1	С	522	GLN	3.7
1	D	229	TRP	3.6
1	D	502	LEU	3.6
1	D	257	LEU	3.6
1	D	240	TRP	3.6
1	D	479	PRO	3.3
1	D	519	ARG	3.3
1	D	283	LYS	3.3
1	D	532	LEU	3.2
1	D	514	ALA	3.2



4AG5

Mol	Chain	Res	Type	RSRZ
1	D	277	TYR	3.1
1	С	277	TYR	3.1
1	D	462	ARG	3.1
1	D	503	ILE	3.0
1	D	482	PRO	2.9
1	С	438	ALA	2.9
1	D	300	PRO	2.9
1	D	486	ALA	2.8
1	D	523	ALA	2.8
1	D	336	TYR	2.8
1	D	448	PHE	2.8
1	D	535	ALA	2.8
1	С	281	CYS	2.8
1	D	236	THR	2.7
1	D	525	LEU	2.7
1	D	244	ALA	2.7
1	D	492	SER	2.6
1	С	427	PHE	2.6
1	D	253	THR	2.5
1	С	275	ARG	2.5
1	D	287	VAL	2.5
1	D	455	TRP	2.5
1	С	286	GLY	2.5
1	D	284	LEU	2.4
1	D	370	VAL	2.4
1	A	550	LEU	2.4
1	D	457	ILE	2.4
1	D	286	GLY	2.4
1	С	425	SER	2.4
1	D	475	MET	2.3
1	С	477	VAL	2.3
1	D	301	LEU	2.2
1	С	498	TYR	2.2
1	D	367	PRO	2.2
1	D	516	GLU	2.2
1	A	219	ARG	2.2
1	D	474	TRP	2.2
1	С	262	TYR	2.2
1	D	429	VAL	2.2
1	D	290	ASN	2.2
1	С	520	TYR	2.2
1	D	241	THR	2.1



Mol	Chain	Res	Type	RSRZ
1	D	279	GLU	2.1
1	D	533	LEU	2.1
1	D	520	TYR	2.1
1	С	519	ARG	2.1
1	С	521	GLY	2.1
1	С	495	ILE	2.1
1	D	453	PHE	2.1
1	А	561	ALA	2.0
1	D	337	LEU	2.0
1	D	526	ASP	2.0
1	D	522	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	GOL	В	1590	6/6	0.65	0.17	$90,\!92,\!93,\!93$	0
3	GOL	А	1590	6/6	0.82	0.16	$68,\!73,\!76,\!76$	0
3	GOL	А	1593	6/6	0.83	0.20	73,79,85,86	0
2	MG	С	1533	1/1	0.84	0.25	77,77,77,77	0
2	MG	В	1588	1/1	0.86	0.11	70,70,70,70	0
2	MG	А	1589	1/1	0.89	0.10	$50,\!50,\!50,\!50$	0
5	SO4	А	1592	5/5	0.91	0.13	114,115,117,118	0
4	ADP	В	1589	27/27	0.94	0.16	45,59,72,74	0
4	ADP	А	1591	27/27	0.96	0.19	38,55,73,74	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers



as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers (i)

There are no such residues in this entry.

