Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:20 PM GMT

PDB ID	:	3QUS
Title	:	Crystal Strucutre of N10-Formyltetrahydrofolate Synthetase with ATPgS
Authors	:	Celeste, L.R.; Chai, G.; Bielak, M.; Lovelace, L.L.; Lebioda, L.
Deposited on	:	2011-02-24
Resolution	:	2.84 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

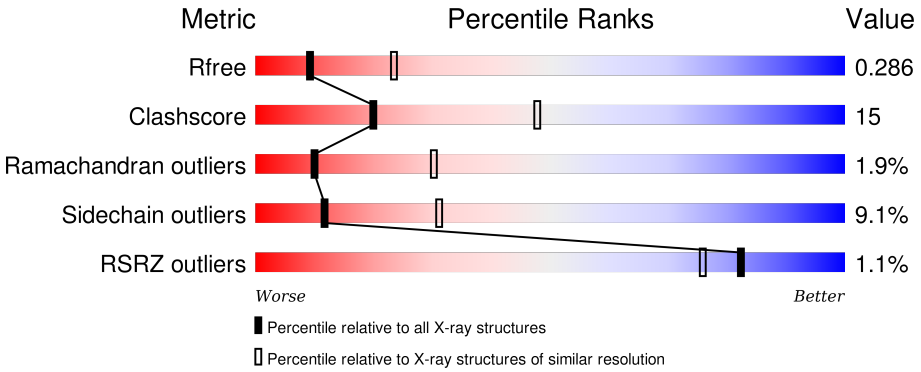
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.84 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3170 (2.88-2.80)
Clashscore	102246	3658 (2.88-2.80)
Ramachandran outliers	100387	3591 (2.88-2.80)
Sidechain outliers	100360	3594 (2.88-2.80)
RSRZ outliers	91569	3184 (2.88-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	557	71% 25%
1	B	557	2% 73% 22%

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
4	TOE	A	701	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8438 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.

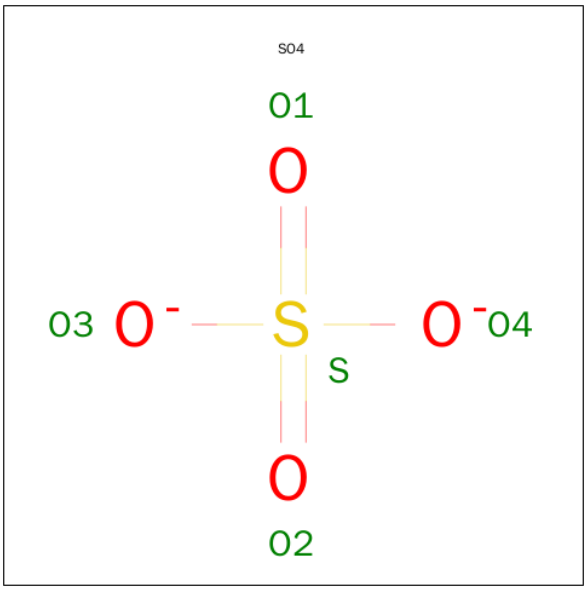
- Molecule 1 is a protein called Formate--tetrahydrofolate ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	0	0
			4100	2596	706	777	21			
1	B	549	Total	C	N	O	S	0	0	0
			3966	2507	680	758	21			

There are 4 discrepancies between the modelled and reference sequences:

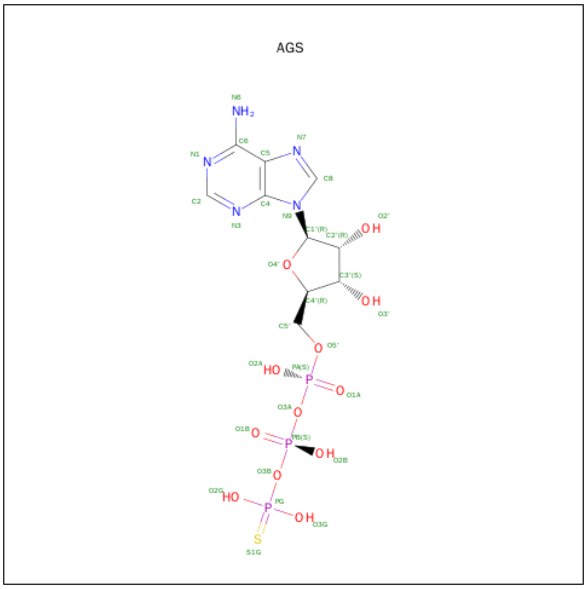
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	DELETION	UNP P21164
A	?	-	VAL	DELETION	UNP P21164
B	?	-	GLU	DELETION	UNP P21164
B	?	-	VAL	DELETION	UNP P21164

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



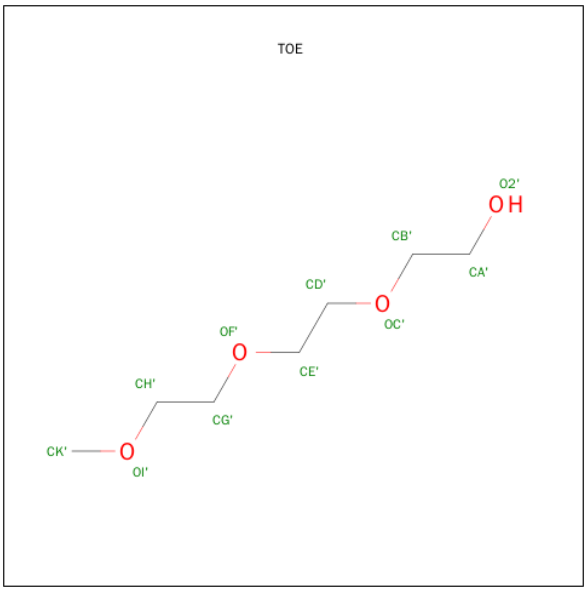
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



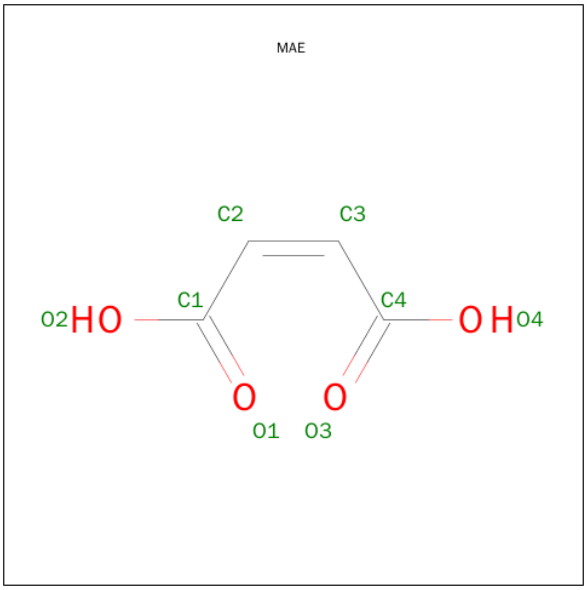
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P S 31 10 5 12 3 1	0	0
3	B	1	Total C N O P S 31 10 5 12 3 1	0	0

- Molecule 4 is 2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXYL (three-letter code: TOE) (formula: $C_7H_{16}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 11 7 4	0	0
4	A	1	Total C O 11 7 4	0	0

- Molecule 5 is MALEIC ACID (three-letter code: MAE) (formula: $C_4H_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 8 4 4	0	0
5	B	1	Total C O 8 4 4	0	0

- Molecule 6 is water.

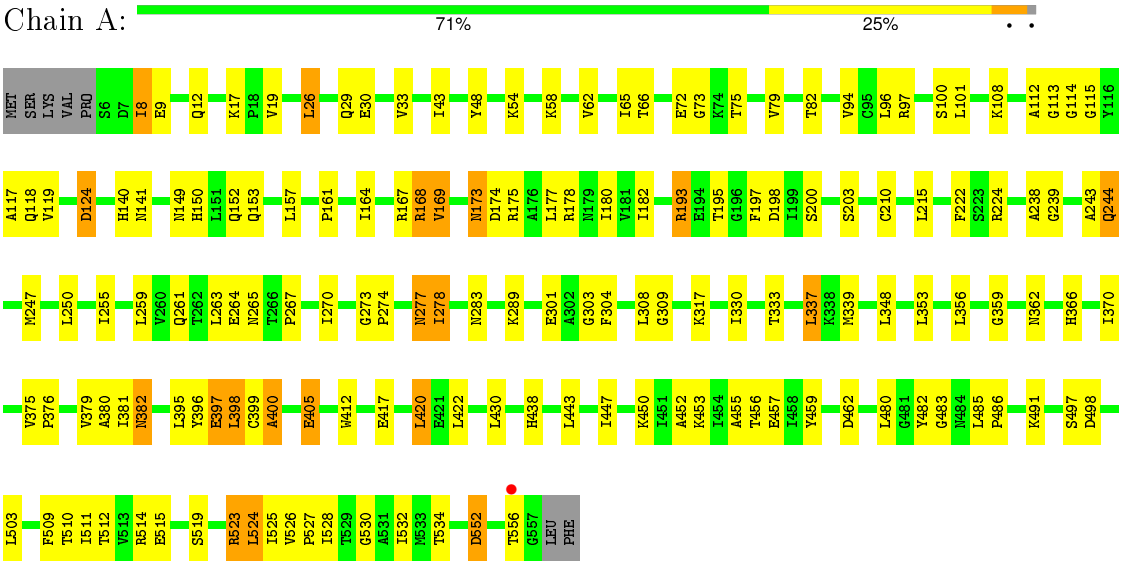
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	173	Total O 173 173	0	0
6	B	69	Total O 69 69	0	0

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

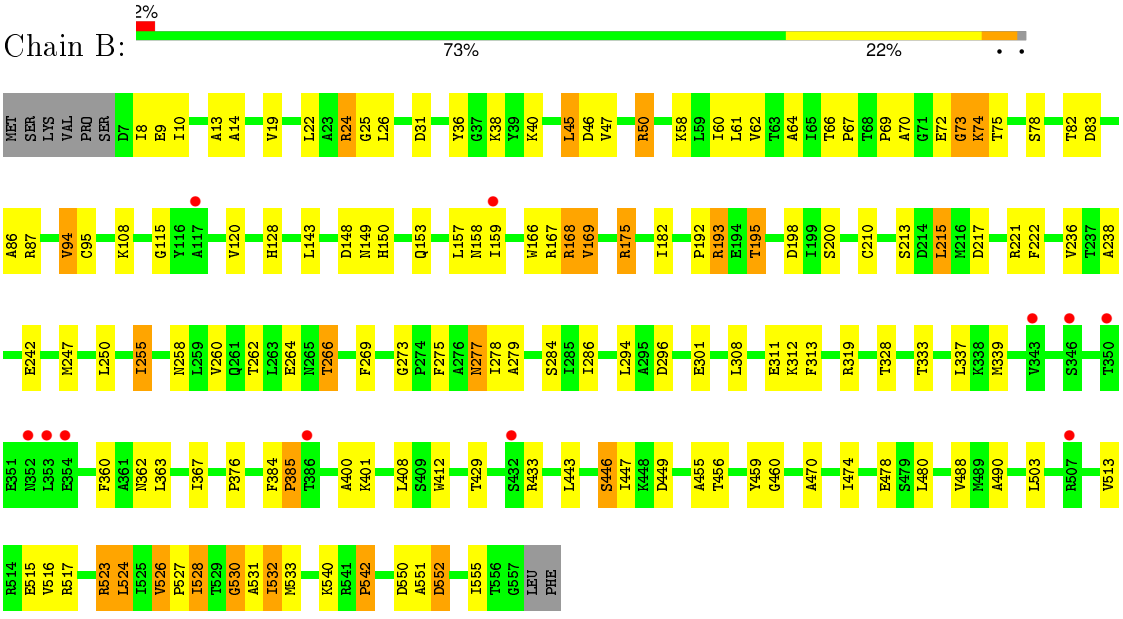
- Molecule 1: Formate--tetrahydrofolate ligase

Chain A:



- Molecule 1: Formate--tetrahydrofolate ligase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	160.84Å 160.84Å 256.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	122.40 – 2.84 48.14 – 2.84	Depositor EDS
% Data completeness (in resolution range)	97.0 (122.40-2.84) 97.0 (48.14-2.84)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.70 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.217 , 0.289 0.216 , 0.286	Depositor DCC
R_{free} test set	1488 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 29567 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	8438	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AGS, MAE, SO4, TOE

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	0.74	1/4168 (0.0%)	0.83	2/5652 (0.0%)
1	B	0.61	3/4034 (0.1%)	0.76	2/5493 (0.0%)
All	All	0.68	4/8202 (0.0%)	0.79	4/11145 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	397	GLU	CG-CD	5.81	1.60	1.51
1	B	412	TRP	C-N	-5.79	1.20	1.34
1	B	408	LEU	C-N	5.54	1.46	1.34
1	B	14	ALA	C-N	5.21	1.46	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	193	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	B	175	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	353	LEU	CA-CB-CG	5.28	127.45	115.30
1	B	128	HIS	N-CA-C	-5.09	97.25	111.00

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	4100	0	4128	132	0
1	B	3966	0	3853	117	0
2	A	20	0	0	1	0
2	B	10	0	0	1	0
3	A	31	0	12	4	0
3	B	31	0	12	6	0
4	A	22	0	32	0	0
5	B	16	0	4	0	0
6	A	173	0	0	12	0
6	B	69	0	0	4	0
All	All	8438	0	8041	240	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 15.

All (240) 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:B:73:GLY:HA2	3:B:700:AGS:S1G	1.52	1.48
1:B:73:GLY:CA	3:B:700:AGS:S1G	2.41	1.07
1:B:523:ARG:HH11	1:B:523:ARG:HG2	0.93	1.07
1:B:262:THR:HG22	1:B:264:GLU:H	1.20	1.01
1:B:277:ASN:ND2	1:B:278:ILE:H	1.56	1.01
1:B:277:ASN:HD22	1:B:278:ILE:N	1.60	0.99
1:A:278:ILE:HG12	1:A:525:ILE:HG21	1.44	0.97
1:A:277:ASN:HD22	1:A:278:ILE:N	1.64	0.95
1:B:523:ARG:NH1	1:B:523:ARG:HG2	1.73	0.94
1:B:75:THR:HB	3:B:700:AGS:O3G	1.67	0.94
1:A:380:ALA:HA	1:A:405:GLU:OE1	1.69	0.93
1:B:523:ARG:HH11	1:B:523:ARG:CG	1.83	0.92
1:B:515:GLU:O	1:B:527:PRO:HD2	1.69	0.90
3:B:700:AGS:O3A	3:B:700:AGS:S1G	2.30	0.89
1:A:277:ASN:ND2	1:A:278:ILE:H	1.70	0.88
1:A:149:ASN:HD21	1:A:153:GLN:HE21	1.21	0.86
1:A:149:ASN:HD22	1:B:175:ARG:NH2	1.76	0.84
1:B:47:VAL:HG11	1:B:294:LEU:HD21	1.60	0.83
1:A:277:ASN:HD22	1:A:278:ILE:H	0.89	0.83
1:B:149:ASN:HD21	1:B:153:GLN:HE21	1.27	0.82
1:A:149:ASN:ND2	1:A:153:GLN:HE21	1.78	0.81
1:A:17:LYS:H	1:A:261:GLN:HE22	1.28	0.81
1:B:516:VAL:HG22	1:B:526:VAL:HG12	1.64	0.79
1:B:9:GLU:HG2	1:B:115:GLY:H	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ARG:HH12	1:B:149:ASN:HD22	1.32	0.77
1:B:169:VAL:HG22	1:B:200:SER:HA	1.64	0.77
1:A:405:GLU:CD	1:A:405:GLU:C	2.43	0.77
1:A:530:GLY:C	1:A:532:ILE:H	1.88	0.76
1:B:150:HIS:HE1	1:B:157:LEU:H	1.35	0.74
1:B:83:ASP:OD2	1:B:262:THR:HG21	1.89	0.73
1:B:45:LEU:HD21	1:B:255:ILE:HG23	1.71	0.71
1:B:169:VAL:CG2	1:B:200:SER:HA	2.21	0.70
1:A:523:ARG:N	1:A:523:ARG:HD3	2.06	0.69
1:A:244:GLN:NE2	1:A:244:GLN:H	1.90	0.69
1:A:452:ALA:O	1:A:456:THR:HB	1.93	0.69
1:A:72:GLU:OE1	3:A:700:AGS:S1G	2.51	0.69
1:B:470:ALA:O	1:B:474:ILE:HG12	1.92	0.68
1:B:337:LEU:HD23	1:B:360:PHE:HA	1.76	0.68
1:A:168:ARG:HG2	1:A:197:PHE:CZ	2.29	0.68
1:A:405:GLU:CD	1:A:405:GLU:O	2.32	0.67
1:A:58:LYS:HE2	6:A:809:HOH:O	1.94	0.67
1:A:173:ASN:N	1:A:173:ASN:HD22	1.91	0.67
1:B:149:ASN:ND2	1:B:153:GLN:HE21	1.93	0.67
1:A:244:GLN:HE21	1:A:244:GLN:H	1.43	0.67
1:B:474:ILE:HD11	1:B:516:VAL:HG21	1.77	0.66
1:B:455:ALA:HA	1:B:459:TYR:CD2	2.30	0.66
1:A:491:LYS:HB3	1:A:528:ILE:HG13	1.77	0.66
1:B:82:THR:HG21	1:B:94:VAL:HG22	1.77	0.66
1:A:54:LYS:HB3	6:A:692:HOH:O	1.97	0.65
1:A:140:HIS:HD2	1:A:203:SER:OG	1.80	0.65
1:B:82:THR:OG1	1:B:94:VAL:HG13	1.97	0.64
1:A:149:ASN:HD22	1:B:175:ARG:HH22	1.46	0.64
1:B:474:ILE:CD1	1:B:516:VAL:HG21	2.28	0.63
1:A:9:GLU:O	1:A:12:GLN:HG2	1.99	0.63
1:A:17:LYS:H	1:A:261:GLN:NE2	1.95	0.62
1:A:43:ILE:CD1	1:A:259:LEU:HB2	2.29	0.62
1:A:43:ILE:HD11	1:A:259:LEU:HB2	1.81	0.62
1:A:17:LYS:N	1:A:261:GLN:HE22	1.97	0.62
1:B:175:ARG:HD3	2:B:602:SO4:O3	2.00	0.62
1:A:149:ASN:HD21	1:A:153:GLN:NE2	1.97	0.61
1:A:447:ILE:HD11	1:A:483:GLY:HA2	1.82	0.61
1:A:167:ARG:NH2	1:A:178:ARG:O	2.34	0.61
1:B:277:ASN:HD22	1:B:278:ILE:H	0.77	0.61
1:B:143:LEU:HD23	1:B:166:TRP:CE2	2.36	0.61
1:A:73:GLY:HA2	3:A:700:AGS:O2B	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LYS:CB	6:A:692:HOH:O	2.48	0.61
1:B:74:LYS:HB3	1:B:301:GLU:OE1	2.00	0.60
1:A:530:GLY:C	1:A:532:ILE:N	2.53	0.60
1:A:528:ILE:HB	6:A:667:HOH:O	2.01	0.60
1:A:512:THR:O	1:A:528:ILE:HG23	2.02	0.59
1:A:405:GLU:O	1:A:405:GLU:OE1	2.20	0.59
1:A:97:ARG:NH1	6:A:784:HOH:O	2.35	0.59
1:A:515:GLU:O	1:A:527:PRO:HD2	2.02	0.59
1:A:380:ALA:HA	1:A:405:GLU:CD	2.22	0.59
1:A:141:ASN:OD1	1:A:168:ARG:HG3	2.04	0.58
1:A:112:ALA:HB1	1:A:119:VAL:O	2.03	0.58
1:B:319:ARG:NE	1:B:443:LEU:HD13	2.18	0.58
1:B:62:VAL:HG11	1:B:78:SER:OG	2.04	0.57
1:A:150:HIS:CE1	1:A:157:LEU:H	2.22	0.57
1:A:169:VAL:HG22	1:A:200:SER:HA	1.85	0.57
1:A:412:TRP:HB3	6:A:621:HOH:O	2.04	0.57
1:B:552:ASP:OD2	1:B:552:ASP:N	2.37	0.57
1:A:150:HIS:HE1	1:A:157:LEU:H	1.51	0.57
1:B:262:THR:HB	1:B:266:THR:H	1.70	0.57
1:B:447:ILE:HG21	1:B:474:ILE:HD12	1.87	0.57
1:B:447:ILE:HD12	1:B:524:LEU:HD22	1.85	0.57
1:A:486:PRO:O	1:A:523:ARG:HB2	2.05	0.56
1:A:337:LEU:O	1:A:359:GLY:HA3	2.05	0.56
1:A:405:GLU:HG3	1:A:422:LEU:HB2	1.87	0.56
1:B:47:VAL:CG1	1:B:294:LEU:HD21	2.35	0.56
1:B:64:ALA:HB2	1:B:74:LYS:HG3	1.87	0.55
1:B:222:PHE:CD1	1:B:247:MET:HB3	2.40	0.55
1:B:182:ILE:O	1:B:192:PRO:HA	2.05	0.55
1:B:74:LYS:HB2	3:B:700:AGS:O1B	2.07	0.55
1:A:150:HIS:CE1	1:A:157:LEU:HB2	2.41	0.55
1:B:312:LYS:HE2	1:B:488:VAL:HG13	1.89	0.55
1:A:491:LYS:HB3	1:A:528:ILE:CG1	2.37	0.55
3:B:700:AGS:O2G	3:B:700:AGS:H5'2	2.07	0.54
1:A:149:ASN:ND2	1:B:175:ARG:HH22	2.06	0.54
1:B:148:ASP:OD2	1:B:168:ARG:NH2	2.30	0.54
1:B:83:ASP:O	1:B:86:ALA:HB3	2.08	0.54
1:B:58:LYS:N	1:B:296:ASP:O	2.37	0.54
1:A:9:GLU:HA	1:A:9:GLU:OE2	2.07	0.54
1:A:239:GLY:HA2	1:A:244:GLN:NE2	2.23	0.53
1:B:523:ARG:NH1	1:B:523:ARG:CG	2.51	0.53
1:B:516:VAL:HG22	1:B:526:VAL:CG1	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ILE:HG12	1:B:236:VAL:HG21	1.90	0.53
1:A:381:ILE:HD12	1:A:395:LEU:HD23	1.90	0.52
1:A:174:ASP:OD2	1:B:168:ARG:NH1	2.42	0.52
1:B:150:HIS:CE1	1:B:157:LEU:H	2.21	0.52
1:B:488:VAL:HG23	1:B:523:ARG:HG3	1.91	0.52
1:B:95:CYS:HA	1:B:269:PHE:O	2.08	0.52
1:A:264:GLU:O	1:A:265:ASN:HB2	2.10	0.52
1:B:62:VAL:HG13	1:B:301:GLU:HB3	1.92	0.51
1:A:82:THR:OG1	1:A:94:VAL:HB	2.10	0.51
1:A:523:ARG:HE	1:A:525:ILE:HD11	1.75	0.51
1:B:550:ASP:O	1:B:552:ASP:N	2.44	0.51
1:B:429:THR:HA	1:B:433:ARG:HE	1.75	0.51
1:B:515:GLU:C	1:B:527:PRO:HD2	2.30	0.51
1:B:550:ASP:C	1:B:552:ASP:H	2.13	0.51
1:B:308:LEU:O	1:B:312:LYS:HG3	2.11	0.51
1:A:75:THR:N	3:A:700:AGS:O1B	2.25	0.51
1:A:277:ASN:ND2	1:A:278:ILE:N	2.43	0.50
1:A:26:LEU:HD11	1:A:267:PRO:HG2	1.94	0.50
1:A:8:ILE:HD11	1:A:114:GLY:HA2	1.94	0.50
1:A:124:ASP:OD1	1:A:124:ASP:N	2.45	0.50
1:A:417:GLU:HA	1:A:420:LEU:HD22	1.92	0.49
1:A:152:GLN:HG2	1:B:175:ARG:NE	2.28	0.49
1:B:13:ALA:HB3	6:B:677:HOH:O	2.12	0.49
1:A:330:ILE:HD11	1:A:366:HIS:HB3	1.94	0.49
1:A:118:GLN:HB2	1:A:263:LEU:HG	1.95	0.49
1:B:456:THR:O	1:B:460:GLY:HA2	2.13	0.49
1:B:31:ASP:HB2	6:B:664:HOH:O	2.12	0.48
1:A:485:LEU:HD13	1:A:523:ARG:HA	1.96	0.48
1:A:73:GLY:CA	3:A:700:AGS:O2B	2.61	0.48
1:A:8:ILE:CD1	1:A:115:GLY:H	2.27	0.48
1:A:124:ASP:HB3	6:A:703:HOH:O	2.14	0.48
1:A:180:ILE:HG22	1:B:182:ILE:HA	1.95	0.48
1:B:66:THR:H	1:B:362:ASN:HD21	1.61	0.48
1:A:149:ASN:ND2	1:B:175:ARG:NH2	2.56	0.48
1:B:384:PHE:CD1	1:B:385:PRO:HD2	2.49	0.48
1:B:429:THR:HA	1:B:433:ARG:NE	2.29	0.48
1:A:48:TYR:CZ	1:A:289:LYS:HD2	2.49	0.48
1:B:488:VAL:CG2	1:B:523:ARG:HG3	2.43	0.47
1:A:239:GLY:HA2	1:A:244:GLN:HE22	1.79	0.47
1:A:66:THR:H	1:A:362:ASN:HD21	1.62	0.47
1:A:330:ILE:HD11	1:A:366:HIS:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:TYR:HB2	1:B:40:LYS:HB2	1.95	0.47
1:B:193:ARG:NH2	1:B:195:THR:CG2	2.77	0.47
1:A:304:PHE:N	2:A:601:SO4:O3	2.46	0.47
1:B:446:SER:O	1:B:447:ILE:C	2.51	0.47
1:A:381:ILE:HD12	1:A:395:LEU:CD2	2.45	0.47
1:A:339:MET:CG	1:A:348:LEU:HD11	2.44	0.47
1:A:149:ASN:HD22	1:B:175:ARG:HH21	1.60	0.47
1:A:405:GLU:HG3	1:A:422:LEU:CB	2.44	0.46
1:B:447:ILE:HG12	1:B:478:GLU:OE2	2.15	0.46
1:B:531:ALA:C	1:B:533:MET:H	2.18	0.46
1:A:317:LYS:HD2	6:A:611:HOH:O	2.14	0.46
1:A:175:ARG:HH12	1:B:149:ASN:ND2	2.06	0.46
1:A:198:ASP:OD1	1:A:534:THR:OG1	2.29	0.46
1:A:398:LEU:C	1:A:400:ALA:H	2.19	0.46
1:B:490:ALA:HB3	1:B:527:PRO:HA	1.98	0.46
1:A:177:LEU:HB3	1:A:197:PHE:HB2	1.98	0.46
1:B:24:ARG:C	1:B:26:LEU:H	2.19	0.46
1:B:46:ASP:O	1:B:50:ARG:HG2	2.16	0.46
1:B:455:ALA:HA	1:B:459:TYR:HD2	1.77	0.46
1:A:482:TYR:O	1:A:524:LEU:HD11	2.16	0.46
1:B:279:ALA:HA	1:B:523:ARG:NH2	2.31	0.45
1:A:149:ASN:O	1:A:153:GLN:HG2	2.17	0.45
1:B:9:GLU:CG	1:B:115:GLY:H	2.25	0.45
1:A:12:GLN:HA	1:A:12:GLN:OE1	2.16	0.45
6:A:568:HOH:O	1:B:168:ARG:HD3	2.16	0.45
1:B:83:ASP:O	1:B:87:ARG:HG2	2.16	0.45
1:B:337:LEU:CD2	1:B:360:PHE:HA	2.46	0.45
1:A:140:HIS:CD2	1:A:203:SER:OG	2.66	0.45
1:B:222:PHE:CE1	1:B:247:MET:HB3	2.52	0.45
1:A:348:LEU:HD23	1:A:348:LEU:HA	1.75	0.45
1:B:446:SER:H	1:B:449:ASP:HB2	1.80	0.45
1:A:308:LEU:HD21	1:A:491:LYS:HG3	1.99	0.45
1:A:161:PRO:HA	1:A:164:ILE:HD12	1.98	0.45
1:B:530:GLY:C	1:B:532:ILE:H	2.16	0.45
1:A:58:LYS:CE	6:A:809:HOH:O	2.57	0.45
1:A:498:ASP:OD2	1:A:511:ILE:HA	2.17	0.45
1:A:75:THR:HA	1:A:301:GLU:OE2	2.17	0.45
1:B:70:ALA:HB2	1:B:339:MET:SD	2.57	0.45
1:A:552:ASP:N	1:A:552:ASP:OD2	2.50	0.44
1:A:222:PHE:O	1:A:238:ALA:HB3	2.18	0.44
1:B:19:VAL:HG22	1:B:38:LYS:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:ARG:NH1	1:B:198:ASP:OD2	2.50	0.44
1:B:531:ALA:C	1:B:533:MET:N	2.71	0.44
1:A:210:CYS:SG	1:A:274:PRO:HD3	2.57	0.44
1:B:528:ILE:HA	1:B:528:ILE:HD12	1.79	0.44
1:A:333:THR:HG22	1:A:382:ASN:HB3	1.99	0.44
1:B:67:PRO:HA	1:B:72:GLU:OE1	2.18	0.44
1:A:405:GLU:OE1	1:A:405:GLU:N	2.51	0.43
1:A:450:LYS:O	1:A:453:LYS:HB2	2.18	0.43
1:B:217:ASP:O	1:B:221:ARG:HG3	2.18	0.43
1:B:143:LEU:HD23	1:B:166:TRP:CZ2	2.53	0.43
1:B:60:ILE:HG22	1:B:60:ILE:O	2.18	0.43
1:B:286:ILE:HG12	6:B:578:HOH:O	2.19	0.43
1:B:210:CYS:HA	1:B:284:SER:HB2	2.00	0.42
1:B:61:LEU:HD13	1:B:313:PHE:CD1	2.54	0.42
1:B:555:ILE:HG12	6:B:647:HOH:O	2.18	0.42
1:B:222:PHE:O	1:B:238:ALA:HB3	2.18	0.42
1:A:96:LEU:O	1:A:270:ILE:HA	2.19	0.42
1:A:54:LYS:HB2	6:A:692:HOH:O	2.15	0.42
1:A:456:THR:HG22	1:A:457:GLU:N	2.34	0.42
1:B:215:LEU:O	1:B:215:LEU:HD22	2.20	0.42
1:B:193:ARG:NH2	1:B:195:THR:HG23	2.33	0.42
1:B:384:PHE:CG	1:B:385:PRO:HD2	2.54	0.42
1:A:447:ILE:HD12	1:A:524:LEU:HD13	2.02	0.42
1:A:447:ILE:CD1	1:A:524:LEU:HD13	2.49	0.42
1:B:193:ARG:HH21	1:B:195:THR:HG23	1.85	0.42
1:A:376:PRO:HA	6:A:619:HOH:O	2.20	0.42
1:A:114:GLY:H	1:A:118:GLN:HG2	1.85	0.41
1:A:303:GLY:O	1:A:309:GLY:HA3	2.20	0.41
1:A:366:HIS:O	1:A:370:ILE:HD12	2.20	0.41
1:A:152:GLN:HG2	1:B:175:ARG:HE	1.84	0.41
1:A:514:ARG:HG3	1:A:528:ILE:O	2.19	0.41
1:B:363:LEU:O	1:B:367:ILE:HG13	2.20	0.41
1:A:523:ARG:HD2	1:A:523:ARG:HH11	1.66	0.41
1:A:43:ILE:HD11	1:A:259:LEU:CB	2.50	0.41
1:A:497:SER:HA	1:A:509:PHE:CE1	2.55	0.41
1:A:255:ILE:HG13	1:A:255:ILE:O	2.20	0.41
1:A:29:GLN:O	1:A:33:VAL:HG23	2.21	0.41
1:A:455:ALA:HA	1:A:459:TYR:CD2	2.56	0.41
1:A:519:SER:O	1:A:523:ARG:N	2.49	0.41
1:A:161:PRO:HA	1:A:164:ILE:CD1	2.51	0.41
1:B:61:LEU:O	1:B:328:THR:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:LYS:O	1:B:542:PRO:HD3	2.21	0.41
1:A:396:TYR:O	1:A:397:GLU:C	2.58	0.41
1:A:379:VAL:HG12	1:A:380:ALA:N	2.36	0.40
1:B:429:THR:HG23	1:B:433:ARG:HD2	2.03	0.40
1:B:515:GLU:HG2	1:B:516:VAL:H	1.86	0.40
1:A:173:ASN:N	1:A:173:ASN:ND2	2.62	0.40
1:A:169:VAL:CG2	1:A:200:SER:HA	2.50	0.40
1:B:531:ALA:O	1:B:533:MET:N	2.54	0.40
1:A:79:VAL:HB	1:A:117:ALA:HB1	2.03	0.40
1:A:65:ILE:CD1	1:A:337:LEU:HD13	2.51	0.40
1:A:243:ALA:O	1:A:247:MET:HG3	2.22	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	548/557 (98%)	494 (90%)	46 (8%)	8 (2%)	13 38
1	B	547/557 (98%)	489 (89%)	45 (8%)	13 (2%)	7 23
All	All	1095/1114 (98%)	983 (90%)	91 (8%)	21 (2%)	10 30

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	400	ALA
1	B	551	ALA
1	A	399	CYS
1	B	108	LYS
1	B	401	LYS
1	B	532	ILE
1	A	8	ILE

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Mol	Chain	Res	Type
1	B	74	LYS
1	B	400	ALA
1	A	556	THR
1	B	73	GLY
1	B	376	PRO
1	A	552	ASP
1	B	25	GLY
1	A	108	LYS
1	A	113	GLY
1	B	69	PRO
1	B	530	GLY
1	B	273	GLY
1	A	273	GLY
1	B	8	ILE

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	419/440 (95%)	382 (91%)	37 (9%)	12	33
1	B	387/440 (88%)	351 (91%)	36 (9%)	11	30
All	All	806/880 (92%)	733 (91%)	73 (9%)	12	31

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	26	LEU
1	A	30	GLU
1	A	62	VAL
1	A	100	SER
1	A	101	LEU
1	A	124	ASP
1	A	168	ARG
1	A	169	VAL

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Mol	Chain	Res	Type
1	A	173	ASN
1	A	182	ILE
1	A	193	ARG
1	A	195	THR
1	A	215	LEU
1	A	224	ARG
1	A	244	GLN
1	A	250	LEU
1	A	277	ASN
1	A	278	ILE
1	A	283	ASN
1	A	337	LEU
1	A	356	LEU
1	A	375	VAL
1	A	382	ASN
1	A	398	LEU
1	A	405	GLU
1	A	420	LEU
1	A	430	LEU
1	A	438	HIS
1	A	443	LEU
1	A	462	ASP
1	A	480	LEU
1	A	503	LEU
1	A	510	THR
1	A	523	ARG
1	A	524	LEU
1	A	526	VAL
1	B	10	ILE
1	B	22	LEU
1	B	24	ARG
1	B	45	LEU
1	B	50	ARG
1	B	94	VAL
1	B	120	VAL
1	B	158	ASN
1	B	168	ARG
1	B	169	VAL
1	B	193	ARG
1	B	195	THR
1	B	213	SER
1	B	215	LEU

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Mol	Chain	Res	Type
1	B	242	GLU
1	B	250	LEU
1	B	255	ILE
1	B	258	ASN
1	B	260	VAL
1	B	266	THR
1	B	275	PHE
1	B	277	ASN
1	B	311	GLU
1	B	333	THR
1	B	385	PRO
1	B	446	SER
1	B	480	LEU
1	B	503	LEU
1	B	513	VAL
1	B	517	ARG
1	B	523	ARG
1	B	524	LEU
1	B	526	VAL
1	B	528	ILE
1	B	542	PRO
1	B	552	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	HIS
1	A	149	ASN
1	A	150	HIS
1	A	173	ASN
1	A	244	GLN
1	A	261	GLN
1	A	265	ASN
1	A	277	ASN
1	A	283	ASN
1	A	362	ASN
1	A	465	ASN
1	B	29	GLN
1	B	149	ASN
1	B	150	HIS
1	B	158	ASN
1	B	179	ASN

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Mol	Chain	Res	Type
1	B	265	ASN
1	B	277	ASN
1	B	362	ASN
1	B	428	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

12 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	SO4	A	601	-	4,4,4	0.60	0	6,6,6	0.27	0
2	SO4	A	603	-	4,4,4	0.15	0	6,6,6	0.22	0
2	SO4	A	604	-	4,4,4	0.12	0	6,6,6	0.29	0
2	SO4	A	605	-	4,4,4	0.12	0	6,6,6	0.22	0
3	AGS	A	700	-	24,33,33	1.37	4 (16%)	28,52,52	2.49	6 (21%)
4	TOE	A	701	-	10,10,10	0.61	0	9,9,9	0.23	0
4	TOE	A	702	-	10,10,10	0.58	0	9,9,9	0.34	0
2	SO4	B	601	-	4,4,4	0.19	0	6,6,6	0.27	0
2	SO4	B	602	-	4,4,4	0.21	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	AGS	B	700	-	24,33,33	1.18	3 (12%)	28,52,52	1.85	4 (14%)
5	MAE	B	702	-	1,7,7	0.45	0	0,8,8	0.00	-
5	MAE	B	703	-	1,7,7	0.65	0	0,8,8	0.00	-

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	SO4	A	601	-	-	0/0/0/0	0/0/0/0
2	SO4	A	603	-	-	0/0/0/0	0/0/0/0
2	SO4	A	604	-	-	0/0/0/0	0/0/0/0
2	SO4	A	605	-	-	0/0/0/0	0/0/0/0
3	AGS	A	700	-	-	0/15/38/38	0/3/3/3
4	TOE	A	701	-	-	0/8/8/8	0/0/0/0
4	TOE	A	702	-	-	0/8/8/8	0/0/0/0
2	SO4	B	601	-	-	0/0/0/0	0/0/0/0
2	SO4	B	602	-	-	0/0/0/0	0/0/0/0
3	AGS	B	700	-	-	0/15/38/38	0/3/3/3
5	MAE	B	702	-	-	0/0/5/5	0/0/0/0
5	MAE	B	703	-	-	0/0/5/5	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	AGS	O4'-C1'	2.02	1.43	1.41
3	A	700	AGS	O4'-C1'	2.34	1.44	1.41
3	A	700	AGS	C2-N3	2.37	1.36	1.32
3	A	700	AGS	PG-S1G	2.58	1.95	1.90
3	B	700	AGS	PG-S1G	2.63	1.95	1.90
3	B	700	AGS	C5-C4	2.88	1.47	1.40
3	A	700	AGS	C5-C4	3.54	1.48	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	700	AGS	PA-O3A-PB	-7.64	111.27	132.73
3	A	700	AGS	N3-C2-N1	-7.13	123.43	128.89
3	B	700	AGS	N3-C2-N1	-6.03	124.28	128.89
3	B	700	AGS	PA-O3A-PB	-4.73	119.44	132.73
3	A	700	AGS	PB-O3B-PG	-3.86	119.74	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	700	AGS	PB-O3B-PG	-3.72	120.18	132.67
3	A	700	AGS	C4'-O4'-C1'	-3.42	105.96	109.72
3	A	700	AGS	C4-C5-N7	-3.13	106.60	109.48
3	B	700	AGS	C4-C5-N7	-2.05	107.59	109.48
3	A	700	AGS	O4'-C1'-N9	3.05	114.48	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	SO4	1	0
3	A	700	AGS	4	0
2	B	602	SO4	1	0
3	B	700	AGS	6	0

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	550/557 (98%)	-0.37	1 (0%)	95	94	9, 14, 43, 58	0
1	B	549/557 (98%)	0.09	11 (2%)	68	59	9, 38, 67, 92	0
All	All	1099/1114 (98%)	-0.14	12 (1%)	82	76	9, 22, 58, 92	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	350	THR	2.8
1	B	343	VAL	2.7
1	B	386	THR	2.7
1	B	117	ALA	2.7
1	B	352	ASN	2.6
1	B	353	LEU	2.4
1	B	346	SER	2.4
1	A	556	THR	2.4
1	B	432	SER	2.3
1	B	507	ARG	2.2
1	B	159	ILE	2.1
1	B	354	GLU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	TOE	A	701	11/11	0.91	0.20	3.10	14,22,32,32	0
3	AGS	B	700	31/31	0.82	0.31	1.93	33,38,41,43	31
3	AGS	A	700	31/31	0.78	0.32	1.85	46,49,49,50	21
5	MAE	B	703	8/8	0.90	0.22	1.65	37,40,42,43	0
2	SO4	A	605	5/5	0.94	0.20	1.56	55,56,57,59	0
2	SO4	B	601	5/5	0.94	0.19	0.47	48,49,50,50	0
2	SO4	A	604	5/5	0.90	0.17	0.27	47,47,49,49	0
2	SO4	B	602	5/5	0.92	0.18	-0.18	44,44,45,46	0
5	MAE	B	702	8/8	0.84	0.18	-0.21	59,60,62,63	0
2	SO4	A	601	5/5	0.99	0.11	-3.05	21,22,23,23	0
4	TOE	A	702	11/11	0.85	0.31	-	34,35,49,49	0
2	SO4	A	603	5/5	0.91	0.20	-	66,66,67,68	0

6.5 Other polymers

There are no such residues in this entry.