



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2017 – 02:33 PM EDT

PDB ID : 3EGJ
Title : N-acetylglucosamine-6-phosphate deacetylase from *Vibrio cholerae*.
Authors : Osipiuk, J.; Maltseva, N.; Stam, J.; Anderson, W.F.; Joachimiak, A.; Center
for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : unknown
Resolution : 2.90 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

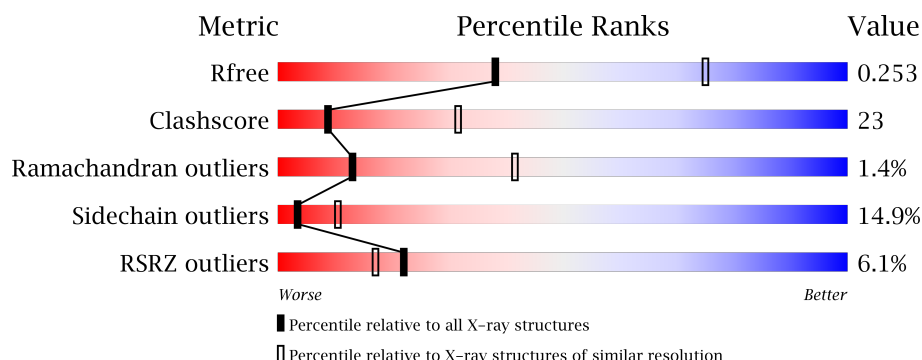
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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 $\leq 5\%$. 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	381	<div> <div>7%</div> <div>57%</div> <div>36%</div> <div>6%</div> </div>
1	B	381	<div> <div>4%</div> <div>57%</div> <div>31%</div> <div>7%</div> <div>5%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5630 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 N-acetylglucosamine-6-phosphate deacetylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			2875	1815	484	557	19			
1	B	361	Total	C	N	O	S	0	0	0
			2728	1719	458	533	18			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP O32445
A	-1	ASN	-	EXPRESSION TAG	UNP O32445
A	0	ALA	-	EXPRESSION TAG	UNP O32445
B	-2	SER	-	EXPRESSION TAG	UNP O32445
B	-1	ASN	-	EXPRESSION TAG	UNP O32445
B	0	ALA	-	EXPRESSION TAG	UNP O32445

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ni	0	0
			1	1		
2	A	1	Total	Ni	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	15	Total	O	0	0
			15	15		

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	77.00 Å 77.00 Å 282.55 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.20 – 2.90 47.14 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.20-2.90) 99.6 (47.14-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.84 (at 2.91 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.189 , 0.247 0.193 , 0.253	Depositor DCC
R_{free} test set	1015 reflections (5.42%)	DCC
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.9	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	0.92	EDS
Total number of atoms	5630	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.71	1/2924 (0.0%)	0.84	1/3964 (0.0%)
1	B	0.76	0/2772	0.85	0/3758
All	All	0.74	1/5696 (0.0%)	0.84	1/7722 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	CYS	CB-SG	-5.95	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	LEU	CA-CB-CG	5.29	127.47	115.30

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	A	2875	0	2876	125	0
1	B	2728	0	2721	130	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	1	0
3	B	5	0	0	0	0
4	B	15	0	0	0	0
All	All	5630	0	5597	253	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 23.

All (253) 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:11:THR:HA	1:B:349:ILE:HG23	1.44	0.99
1:B:3:ALA:HB2	1:B:41:MET:HE2	1.41	0.97
1:A:98:THR:HB	1:A:130:PRO:HA	1.46	0.96
1:B:357:LEU:HB2	1:B:370:VAL:HG13	1.47	0.96
1:A:272:THR:HG21	1:A:282:PHE:CZ	1.99	0.95
1:B:3:ALA:HB2	1:B:41:MET:CE	2.00	0.91
1:B:344:GLU:O	1:B:353:MET:CE	2.20	0.90
1:B:60:LEU:O	1:B:95:THR:HG23	1.77	0.85
1:A:93:LEU:O	1:A:95:THR:HG22	1.78	0.84
1:B:297:VAL:HA	1:B:302:THR:O	1.77	0.84
1:B:98:THR:HG21	1:B:104:MET:CE	2.07	0.83
1:B:60:LEU:H	1:B:95:THR:CG2	1.92	0.82
1:B:120:ASN:HD21	1:B:354:ILE:HD13	1.43	0.80
1:A:93:LEU:O	1:A:95:THR:CG2	2.30	0.80
1:B:98:THR:HG21	1:B:104:MET:HE2	1.63	0.80
1:B:93:LEU:O	1:B:95:THR:HG22	1.82	0.80
1:B:95:THR:HB	1:B:126:HIS:HB3	1.64	0.78
1:B:120:ASN:ND2	1:B:354:ILE:HD13	1.98	0.78
1:B:376:GLU:O	1:B:377:GLN:HB2	1.83	0.77
1:A:236:PRO:HG2	1:A:237:GLU:OE2	1.86	0.76
1:B:201:ARG:HG2	1:B:201:ARG:HH11	1.50	0.76
1:B:344:GLU:O	1:B:353:MET:HE2	1.85	0.76
1:A:58:LEU:HD21	1:A:340:ILE:HD13	1.66	0.75
1:A:272:THR:CG2	1:A:282:PHE:CZ	2.71	0.74
1:B:67:MET:CE	1:B:272:THR:HB	2.19	0.73
1:B:84:ASN:HB3	1:B:89:CYS:HB3	1.68	0.73
1:A:370:VAL:HA	1:A:374:GLN:O	1.88	0.73
1:A:272:THR:HG22	1:A:274:PRO:HD2	1.70	0.72
1:A:80:MET:HE2	1:A:92:PHE:HE1	1.55	0.72
1:B:357:LEU:HB2	1:B:370:VAL:CG1	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:VAL:HG11	1:B:329:LEU:HD23	1.72	0.71
1:A:60:LEU:H	1:A:95:THR:CG2	2.03	0.71
1:A:148:SER:HB2	1:A:153:ILE:HD11	1.72	0.71
1:B:309:THR:HG22	1:B:312:GLU:H	1.53	0.71
1:A:4:LEU:O	1:A:20:ALA:HB1	1.92	0.70
1:B:67:MET:HE1	1:B:272:THR:HB	1.74	0.70
1:A:84:ASN:HB3	1:A:89:CYS:HB3	1.73	0.69
1:B:174:LYS:HB3	1:B:176:GLU:HG2	1.75	0.69
1:B:344:GLU:O	1:B:353:MET:HE1	1.91	0.69
1:A:58:LEU:CD2	1:A:340:ILE:HD13	2.23	0.68
1:B:298:ASP:HB2	1:B:300:ASN:HB2	1.74	0.68
1:A:111:ALA:O	1:A:115:GLN:HG2	1.94	0.68
1:A:120:ASN:HD21	1:A:354:ILE:HD13	1.57	0.68
1:B:272:THR:HG21	1:B:284:PHE:CE1	2.29	0.68
1:A:80:MET:HE2	1:A:92:PHE:CE1	2.29	0.67
1:B:60:LEU:H	1:B:95:THR:HG23	1.60	0.67
1:A:309:THR:HG22	1:A:312:GLU:CG	2.26	0.66
1:B:201:ARG:CG	1:B:201:ARG:HH11	2.09	0.66
1:A:65:GLY:HA2	1:A:279:MET:HE1	1.76	0.66
1:B:267:LEU:HD11	1:B:317:THR:HG21	1.78	0.65
1:B:313:ALA:O	1:B:317:THR:HG23	1.96	0.65
1:A:128:GLU:OE2	1:A:140:HIS:NE2	2.20	0.65
1:A:98:THR:HG23	1:A:140:HIS:CD2	2.32	0.65
1:B:213:HIS:HB2	1:B:216:ASN:HD22	1.59	0.65
1:B:219:THR:HG22	1:B:227:GLY:HA3	1.77	0.64
1:A:248:HIS:CD2	1:A:303:LEU:HD21	2.33	0.64
1:A:98:THR:CG2	1:A:140:HIS:HD2	2.10	0.64
1:B:219:THR:HB	1:B:228:VAL:HG23	1.79	0.64
1:B:356:ASN:HA	1:B:370:VAL:O	1.98	0.64
1:A:120:ASN:ND2	1:A:354:ILE:HD13	2.14	0.63
1:A:60:LEU:H	1:A:95:THR:HG21	1.64	0.63
1:B:98:THR:HG21	1:B:104:MET:HE3	1.80	0.63
1:A:348:ARG:HB3	1:A:353:MET:SD	2.39	0.63
1:A:214:LEU:O	1:A:215:PHE:HB2	1.98	0.63
1:A:59:GLN:HA	1:A:95:THR:HG21	1.80	0.63
1:B:100:SER:HB2	1:B:102:GLU:OE2	1.98	0.62
1:A:24:ASN:HB3	1:A:29:GLU:CG	2.29	0.62
1:A:178:ILE:O	1:A:182:VAL:HG23	2.00	0.62
1:A:91:SER:HB3	1:A:123:LEU:HD11	1.80	0.62
1:B:284:PHE:O	1:B:285:VAL:C	2.38	0.62
1:B:1:MET:HG2	1:B:24:ASN:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:THR:CG2	1:B:104:MET:HE3	2.32	0.60
1:B:376:GLU:O	1:B:377:GLN:CB	2.50	0.60
1:B:242:ILE:HD13	1:B:254:ILE:HG23	1.82	0.60
1:B:112:ARG:HA	1:B:162:VAL:HG11	1.84	0.60
1:A:317:THR:O	1:A:321:VAL:HB	2.03	0.59
1:A:75:GLU:O	1:A:79:THR:HG22	2.03	0.59
1:B:60:LEU:H	1:B:95:THR:HG21	1.68	0.59
1:B:22:ILE:O	1:B:22:ILE:HG13	2.02	0.59
1:A:357:LEU:HB2	1:A:370:VAL:HG13	1.84	0.59
1:B:3:ALA:CB	1:B:41:MET:HE2	2.25	0.59
1:A:298:ASP:O	1:A:300:ASN:N	2.36	0.59
1:B:197:TYR:CZ	1:B:201:ARG:HD2	2.38	0.58
1:B:201:ARG:HG2	1:B:201:ARG:NH1	2.15	0.58
1:A:213:HIS:ND1	1:A:216:ASN:HB2	2.18	0.58
1:B:112:ARG:HH22	1:B:161:ASP:CG	2.07	0.58
1:B:170:PRO:C	1:B:172:ASN:H	2.06	0.58
1:B:117:LYS:HE3	1:B:118:TYR:CE2	2.39	0.58
1:A:131:TYR:HA	1:A:146:ARG:O	2.04	0.57
1:A:123:LEU:H	1:A:123:LEU:HD12	1.67	0.57
1:B:186:ILE:HG22	1:B:187:VAL:N	2.19	0.57
1:A:23:ILE:HD13	1:A:373:GLY:HA2	1.86	0.57
1:A:76:THR:O	1:A:80:MET:HG3	2.05	0.57
1:B:182:VAL:HG21	1:B:207:GLY:HA3	1.86	0.57
1:B:213:HIS:ND1	1:B:216:ASN:HB2	2.19	0.57
1:B:221:MET:HB2	1:B:229:VAL:HG22	1.86	0.57
1:A:9:ILE:O	1:A:15:VAL:HA	2.05	0.57
1:A:62:GLY:HA2	1:A:80:MET:SD	2.45	0.57
1:A:98:THR:HB	1:A:130:PRO:CA	2.27	0.56
1:A:60:LEU:H	1:A:95:THR:HG23	1.70	0.56
1:B:343:ASP:HA	1:B:346:LEU:O	2.05	0.56
1:B:102:GLU:H	1:B:102:GLU:CD	2.07	0.56
1:B:267:LEU:HD22	1:B:313:ALA:HB1	1.86	0.56
1:A:272:THR:HG21	1:A:282:PHE:HZ	1.65	0.56
1:A:18:LYS:O	1:A:18:LYS:HG2	2.06	0.56
1:A:309:THR:HG22	1:A:312:GLU:HB2	1.88	0.56
1:A:189:SER:OG	1:A:212:THR:HG23	2.05	0.56
1:B:71:GLU:HB3	1:B:76:THR:HG1	1.70	0.56
1:A:24:ASN:HB3	1:A:29:GLU:HG2	1.88	0.55
1:B:67:MET:HE2	1:B:272:THR:HB	1.88	0.55
1:B:377:GLN:HA	1:B:377:GLN:NE2	2.22	0.55
1:B:73:THR:HG23	1:B:76:THR:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:GLY:O	1:A:373:GLY:HA3	2.07	0.55
1:B:203:SER:HB2	1:B:208:ILE:HD12	1.88	0.54
1:B:3:ALA:HB3	1:B:43:VAL:HG12	1.90	0.54
1:A:123:LEU:HD12	1:A:123:LEU:N	2.22	0.54
1:B:59:GLN:HA	1:B:95:THR:HG21	1.90	0.54
1:A:24:ASN:HB3	1:A:29:GLU:HG3	1.89	0.54
1:A:309:THR:HG22	1:A:312:GLU:CB	2.38	0.54
1:B:24:ASN:HB3	1:B:29:GLU:HG3	1.89	0.53
1:A:321:VAL:HG12	1:A:323:ILE:HG13	1.89	0.53
1:B:1:MET:CG	1:B:24:ASN:HB2	2.39	0.53
1:B:258:HIS:HA	1:B:265:LEU:HD12	1.91	0.52
1:A:93:LEU:O	1:A:95:THR:HG23	2.06	0.52
1:B:221:MET:HA	1:B:226:PRO:O	2.09	0.52
1:A:290:TYR:HE2	1:A:299:GLU:HB3	1.74	0.52
1:B:266:VAL:HG13	1:B:336:PRO:HG3	1.92	0.52
1:A:33:PRO:HB2	1:A:35:GLU:OE2	2.09	0.52
1:B:219:THR:HG22	1:B:227:GLY:CA	2.39	0.52
1:A:124:GLY:HA3	1:A:164:ALA:HB2	1.92	0.52
1:A:34:ILE:HG23	1:A:35:GLU:H	1.74	0.52
1:B:377:GLN:HA	1:B:377:GLN:HE21	1.74	0.52
1:B:115:GLN:HE22	1:B:124:GLY:HA2	1.75	0.51
1:B:-1:ASN:HD22	1:B:0:ALA:N	2.08	0.51
1:B:302:THR:HG22	1:B:303:LEU:N	2.25	0.51
1:B:22:ILE:HB	1:B:41:MET:CE	2.41	0.51
1:B:22:ILE:HB	1:B:41:MET:HE3	1.92	0.51
1:B:57:ASP:HB2	1:B:310:MET:SD	2.50	0.51
1:A:98:THR:CG2	1:A:140:HIS:CD2	2.90	0.51
1:A:24:ASN:CB	1:A:29:GLU:HG3	2.40	0.51
1:A:75:GLU:O	1:A:79:THR:CG2	2.59	0.50
1:B:186:ILE:CG2	1:B:187:VAL:N	2.73	0.50
1:B:298:ASP:HB2	1:B:300:ASN:H	1.75	0.50
1:B:370:VAL:HA	1:B:374:GLN:O	2.12	0.50
1:A:148:SER:OG	1:A:173:ASN:HB3	2.12	0.50
1:A:219:THR:HB	1:A:228:VAL:H	1.75	0.50
1:A:103:ASN:HA	1:A:106:GLN:HE21	1.78	0.49
1:A:248:HIS:NE2	1:A:303:LEU:HD21	2.26	0.49
1:A:67:MET:HE1	1:A:272:THR:HA	1.94	0.49
1:B:112:ARG:NH2	1:B:161:ASP:OD1	2.46	0.49
1:A:133:ASN:ND2	1:A:194:ASN:HB3	2.26	0.49
1:A:34:ILE:HG23	1:A:35:GLU:N	2.28	0.49
1:B:64:GLY:HA2	1:B:277:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LYS:HG2	1:A:34:ILE:HG22	1.93	0.49
1:B:21:VAL:HG11	1:B:349:ILE:HD11	1.94	0.49
1:A:174:LYS:HE3	1:A:177:HIS:CE1	2.48	0.48
1:A:71:GLU:HB3	1:A:76:THR:HG1	1.78	0.48
1:A:327:GLU:OE1	1:A:327:GLU:HA	2.12	0.48
1:B:-1:ASN:C	1:B:-1:ASN:HD22	2.16	0.48
1:B:291:TYR:CE1	1:B:294:GLY:HA2	2.49	0.48
1:B:98:THR:CG2	1:B:104:MET:CE	2.85	0.48
1:A:189:SER:HA	1:A:210:PHE:O	2.13	0.48
1:A:85:LEU:HD22	1:A:369:THR:HG21	1.96	0.48
1:A:279:MET:HB2	1:A:279:MET:HE3	1.79	0.48
1:A:224:ARG:NH2	3:A:403:SO4:O2	2.34	0.48
1:A:173:ASN:N	1:A:173:ASN:ND2	2.62	0.47
1:B:210:PHE:CD2	1:B:211:ALA:N	2.82	0.47
1:A:127:LEU:HB2	1:A:166:VAL:HG22	1.96	0.47
1:B:309:THR:HG23	1:B:311:ILE:HG22	1.96	0.47
1:A:130:PRO:HG3	1:A:146:ARG:CZ	2.44	0.47
1:B:174:LYS:O	1:B:177:HIS:HB2	2.15	0.47
1:B:289:VAL:HG21	1:B:296:CYS:HB3	1.97	0.47
1:A:98:THR:HG22	1:A:129:GLY:HA3	1.97	0.46
1:A:60:LEU:O	1:A:95:THR:HG23	2.15	0.46
1:B:44:VAL:HG12	1:B:46:LEU:HD23	1.97	0.46
1:A:282:PHE:CE2	1:A:289:VAL:HB	2.51	0.46
1:B:170:PRO:C	1:B:172:ASN:N	2.69	0.46
1:A:117:LYS:HE3	1:A:117:LYS:HB2	1.68	0.45
1:A:135:MET:HE2	1:A:194:ASN:HD22	1.81	0.45
1:A:60:LEU:HD13	1:A:271:ALA:HB3	1.98	0.45
1:B:201:ARG:NH1	1:B:235:THR:OG1	2.49	0.45
1:A:23:ILE:CD1	1:A:373:GLY:HA2	2.47	0.45
1:A:8:LYS:NZ	1:B:319:GLU:HG2	2.32	0.45
1:A:126:HIS:CE1	1:A:165:LYS:HD3	2.51	0.45
1:A:130:PRO:HG3	1:A:146:ARG:NH2	2.33	0.44
1:B:213:HIS:HE1	1:B:217:ALA:HB3	1.82	0.44
1:B:53:PRO:HG3	1:B:349:ILE:HG22	1.99	0.44
1:A:127:LEU:HD23	1:A:127:LEU:HA	1.77	0.44
1:A:73:THR:HG23	1:A:76:THR:H	1.82	0.44
1:A:131:TYR:OH	1:A:152:MET:HB3	2.18	0.44
1:A:133:ASN:OD1	1:A:135:MET:HG2	2.18	0.44
1:A:119:PRO:O	1:A:121:GLN:HG3	2.18	0.44
1:A:318:VAL:CG2	1:A:325:LEU:HA	2.47	0.44
1:A:65:GLY:HA2	1:A:279:MET:CE	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:MET:O	1:B:43:VAL:HG13	2.18	0.44
1:B:4:LEU:CD1	1:B:357:LEU:HD23	2.48	0.44
1:B:309:THR:CG2	1:B:311:ILE:HG22	2.48	0.43
1:A:149:ASP:OD2	1:A:151:THR:HB	2.18	0.43
1:A:171:GLU:OE1	1:A:193:THR:OG1	2.31	0.43
1:A:290:TYR:HB3	1:A:292:ARG:HH11	1.83	0.43
1:B:21:VAL:HB	1:B:31:VAL:HG22	2.01	0.43
1:A:272:THR:HB	1:A:306:SER:O	2.18	0.43
1:B:157:CYS:SG	1:B:181:LEU:HD23	2.58	0.43
1:B:168:LEU:C	1:B:168:LEU:HD12	2.38	0.43
1:A:152:MET:O	1:A:156:ILE:HG13	2.19	0.43
1:A:309:THR:HG23	1:A:312:GLU:H	1.84	0.43
1:B:333:THR:C	1:B:336:PRO:HD2	2.39	0.43
1:B:76:THR:O	1:B:80:MET:HG2	2.19	0.43
1:A:177:HIS:O	1:A:181:LEU:HG	2.18	0.43
1:A:167:THR:OG1	1:A:212:THR:HG21	2.19	0.43
1:B:6:ASN:OD1	1:B:48:GLY:N	2.51	0.43
1:B:169:ALA:HB1	1:B:171:GLU:OE1	2.19	0.42
1:B:228:VAL:O	1:B:229:VAL:C	2.56	0.42
1:A:148:SER:HB2	1:A:153:ILE:CD1	2.48	0.42
1:A:273:ALA:HB3	1:A:274:PRO:HD3	2.01	0.42
1:A:309:THR:HG22	1:A:312:GLU:HG3	1.98	0.42
1:B:188:VAL:O	1:B:208:ILE:HG23	2.20	0.42
1:A:32:CYS:HB2	1:A:33:PRO:CD	2.50	0.42
1:B:21:VAL:HG11	1:B:349:ILE:CD1	2.50	0.42
1:B:359:VAL:HG22	1:B:367:LYS:HB2	2.01	0.42
1:A:114:TYR:OH	1:A:121:GLN:NE2	2.53	0.42
1:B:251:TYR:HA	1:B:254:ILE:HG13	2.02	0.42
1:B:376:GLU:HB3	1:B:377:GLN:H	1.78	0.42
1:A:151:THR:O	1:A:154:ASP:HB2	2.20	0.42
1:A:55:PHE:N	1:A:55:PHE:CD1	2.86	0.42
1:B:67:MET:HE2	1:B:273:ALA:H	1.85	0.42
1:B:60:LEU:C	1:B:95:THR:HG23	2.39	0.42
1:A:21:VAL:HG22	1:A:23:ILE:HG22	2.01	0.42
1:B:334:LEU:HD13	1:B:348:ARG:HG3	2.01	0.42
1:B:71:GLU:HB3	1:B:76:THR:OG1	2.20	0.41
1:B:174:LYS:HD3	1:B:177:HIS:CE1	2.55	0.41
1:B:335:TYR:N	1:B:335:TYR:CD1	2.86	0.41
1:A:362:ARG:NH2	1:B:362:ARG:NH1	2.68	0.41
1:B:80:MET:O	1:B:81:HIS:C	2.57	0.41
1:B:18:LYS:HG2	1:B:18:LYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:MET:O	1:B:313:ALA:HB3	2.20	0.41
1:B:73:THR:CG2	1:B:76:THR:OG1	2.69	0.41
1:A:82:LYS:H	1:A:82:LYS:HG2	1.67	0.41
1:A:309:THR:HG22	1:A:312:GLU:OE2	2.20	0.41
1:B:183:LYS:HE3	1:B:183:LYS:HB2	1.79	0.41
1:A:157:CYS:SG	1:A:181:LEU:HD23	2.61	0.41
1:A:176:GLU:N	1:A:176:GLU:OE2	2.37	0.41
1:A:335:TYR:N	1:A:335:TYR:CD1	2.88	0.41
1:A:87:SER:CB	1:A:309:THR:OG1	2.68	0.41
1:B:112:ARG:CA	1:B:162:VAL:HG11	2.50	0.41
1:B:367:LYS:O	1:B:377:GLN:NE2	2.54	0.41
1:A:130:PRO:HG2	1:A:131:TYR:CD1	2.56	0.40
1:A:245:ASP:HB3	1:A:308:LEU:HD22	2.02	0.40
1:B:258:HIS:CA	1:B:265:LEU:HD12	2.51	0.40
1:A:71:GLU:HB3	1:A:76:THR:OG1	2.20	0.40
1:B:289:VAL:CG2	1:B:296:CYS:HB3	2.51	0.40
1:B:331:MET:HA	1:B:335:TYR:CD2	2.56	0.40
1:A:59:GLN:HG2	1:A:270:ASP:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	377/381 (99%)	341 (90%)	30 (8%)	6 (2%)	11	37
1	B	357/381 (94%)	335 (94%)	18 (5%)	4 (1%)	17	48
All	All	734/762 (96%)	676 (92%)	48 (6%)	10 (1%)	13	41

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	ALA
1	A	285	VAL
1	A	299	GLU
1	B	285	VAL
1	B	34	ILE
1	A	35	GLU
1	B	213	HIS
1	A	63	CYS
1	A	213	HIS
1	B	171	GLU

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	310/312 (99%)	260 (84%)	50 (16%)	3	8
1	B	293/312 (94%)	253 (86%)	40 (14%)	4	12
All	All	603/624 (97%)	513 (85%)	90 (15%)	3	10

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	ASN
1	A	1	MET
1	A	4	LEU
1	A	5	THR
1	A	15	VAL
1	A	16	LEU
1	A	18	LYS
1	A	21	VAL
1	A	23	ILE
1	A	35	GLU
1	A	41	MET
1	A	43	VAL
1	A	67	MET
1	A	70	ASP

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Mol	Chain	Res	Type
1	A	79	THR
1	A	82	LYS
1	A	95	THR
1	A	98	THR
1	A	99	SER
1	A	115	GLN
1	A	122	SER
1	A	123	LEU
1	A	135	MET
1	A	139	ILE
1	A	140	HIS
1	A	142	VAL
1	A	143	ASP
1	A	183	LYS
1	A	198	SER
1	A	201	ARG
1	A	205	GLU
1	A	229	VAL
1	A	238	VAL
1	A	249	VAL
1	A	268	VAL
1	A	272	THR
1	A	278	GLU
1	A	284	PHE
1	A	288	LYS
1	A	292	ARG
1	A	302	THR
1	A	334	LEU
1	A	344	GLU
1	A	357	LEU
1	A	359	VAL
1	A	362	ARG
1	A	369	THR
1	A	370	VAL
1	A	374	GLN
1	A	377	GLN
1	B	-1	ASN
1	B	18	LYS
1	B	21	VAL
1	B	22	ILE
1	B	24	ASN
1	B	29	GLU

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Mol	Chain	Res	Type
1	B	37	LEU
1	B	39	SER
1	B	41	MET
1	B	73	THR
1	B	87	SER
1	B	95	THR
1	B	98	THR
1	B	99	SER
1	B	125	LEU
1	B	149	ASP
1	B	150	ASP
1	B	171	GLU
1	B	174	LYS
1	B	198	SER
1	B	201	ARG
1	B	202	LYS
1	B	249	VAL
1	B	254	ILE
1	B	263	GLU
1	B	265	LEU
1	B	268	VAL
1	B	278	GLU
1	B	284	PHE
1	B	288	LYS
1	B	289	VAL
1	B	298	ASP
1	B	309	THR
1	B	345	LYS
1	B	349	ILE
1	B	354	ILE
1	B	357	LEU
1	B	359	VAL
1	B	370	VAL
1	B	377	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-1	ASN
1	A	19	HIS
1	A	24	ASN
1	A	103	ASN

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Mol	Chain	Res	Type
1	A	106	GLN
1	A	115	GLN
1	A	120	ASN
1	A	121	GLN
1	A	126	HIS
1	A	172	ASN
1	A	194	ASN
1	A	315	GLN
1	A	372	ASN
1	B	-1	ASN
1	B	24	ASN
1	B	115	GLN
1	B	121	GLN
1	B	172	ASN
1	B	173	ASN
1	B	177	HIS
1	B	216	ASN
1	B	377	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
3	SO4	A	403	-	4,4,4	0.09	0	6,6,6	0.48	0
3	SO4	B	404	-	4,4,4	0.15	0	6,6,6	0.16	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
3	SO4	A	403	-	-	0/0/0/0	0/0/0/0
3	SO4	B	404	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	SO4	1	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, 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	379/381 (99%)	0.16	28 (7%) 15 11	17, 29, 56, 70	0
1	B	361/381 (94%)	0.04	17 (4%) 32 28	19, 29, 54, 60	0
All	All	740/762 (97%)	0.10	45 (6%) 22 17	17, 29, 54, 70	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	VAL	5.3
1	A	143	ASP	4.4
1	A	286	GLY	4.1
1	B	281	TYR	4.0
1	A	139	ILE	3.9
1	A	-1	ASN	3.8
1	B	288	LYS	3.7
1	A	289	VAL	3.7
1	A	297	VAL	3.7
1	A	144	PHE	3.6
1	B	285	VAL	3.6
1	A	300	ASN	3.2
1	B	290	TYR	3.2
1	B	283	ILE	3.1
1	B	297	VAL	3.0
1	A	280	ASP	3.0
1	B	284	PHE	2.9
1	A	283	ILE	2.9
1	B	298	ASP	2.8
1	A	141	SER	2.8
1	A	285	VAL	2.8
1	A	138	GLY	2.6
1	B	286	GLY	2.6
1	B	299	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	299	GLU	2.4
1	B	300	ASN	2.3
1	A	290	TYR	2.3
1	A	303	LEU	2.3
1	B	296	CYS	2.2
1	A	292	ARG	2.2
1	A	39	SER	2.2
1	B	287	LYS	2.2
1	A	298	ASP	2.2
1	B	282	PHE	2.2
1	A	38	PRO	2.2
1	A	140	HIS	2.2
1	A	281	TYR	2.2
1	B	130	PRO	2.1
1	B	293	ASP	2.1
1	A	0	ALA	2.1
1	A	37	LEU	2.1
1	B	280	ASP	2.1
1	A	40	GLU	2.1
1	A	2	TYR	2.0
1	A	135	MET	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. 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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	NI	A	401	1/1	0.83	0.19	0.05	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NI	B	402	1/1	0.89	0.13	-2.14	93,93,93,93	0
3	SO4	B	404	5/5	0.96	0.20	-	61,62,62,62	5
3	SO4	A	403	5/5	0.97	0.21	-	49,49,50,50	5

6.5 Other polymers [i](#)

There are no such residues in this entry.