



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 10:48 PM EDT

PDB ID : 3HNO
Title : Crystal Structure of Pyrophosphate-dependent phosphofructokinase from *Nitrosospira multiformis*. Northeast Structural Genomics Consortium target id NmR42
Authors : Seetharaman, J.; Abashidze, M.; Sahdev, S.; Janjua, H.; Xiao, R.; Ciccocanti, C.; Foote, E.L.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2009-05-31
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

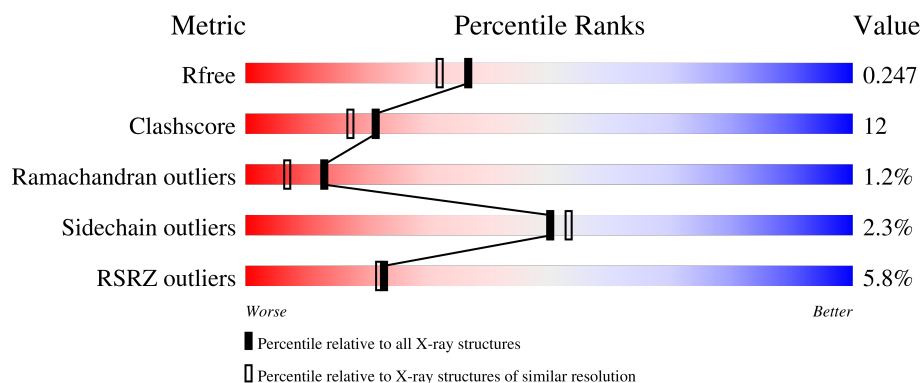
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


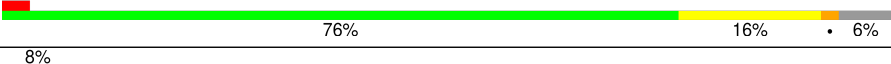
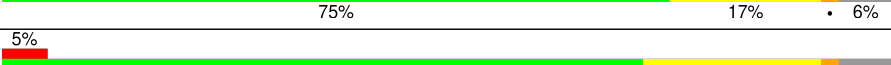

The reported resolution of this entry is 2.00 Å.

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	419	 6% 77% 16% • 6%
1	B	419	 3% 76% 16% • 6%
1	C	419	 8% 75% 17% • 6%
1	D	419	 5% 72% 20% • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12308 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 Pyrophosphate-dependent phosphofructokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			2965	1886	502	562	15			
1	B	395	Total	C	N	O	S	0	0	0
			2965	1886	502	562	15			
1	C	395	Total	C	N	O	S	0	1	0
			2970	1890	502	562	16			
1	D	394	Total	C	N	O	S	0	1	0
			2966	1888	501	561	16			

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Br	0	0
			1	1		

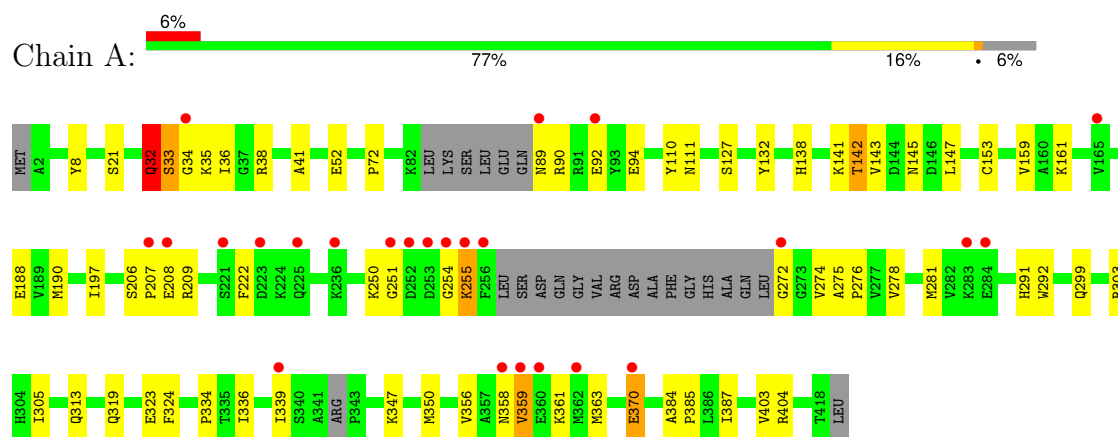
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	94	Total	O	0	0
			94	94		
3	B	130	Total	O	0	0
			130	130		
3	C	89	Total	O	0	0
			89	89		
3	D	128	Total	O	0	0
			128	128		

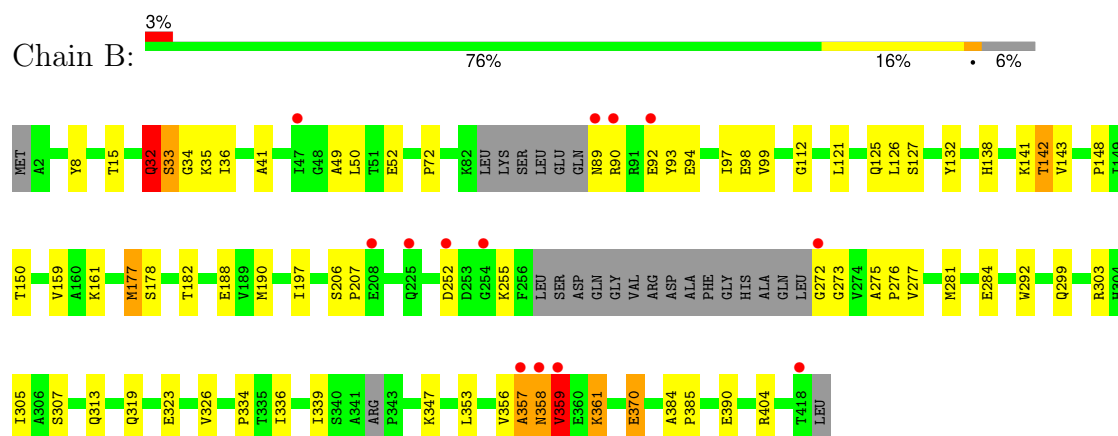
3 Residue-property plots [i](#)

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.

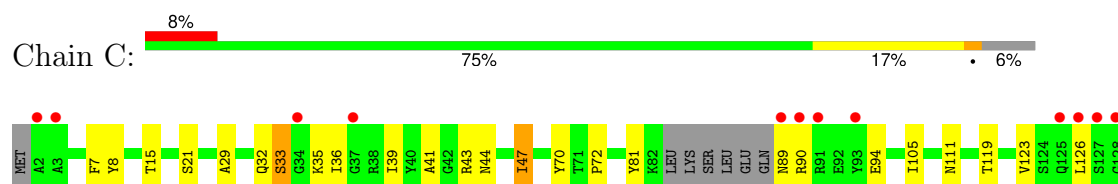
- Molecule 1: Pyrophosphate-dependent phosphofructokinase



- Molecule 1: Pyrophosphate-dependent phosphofructokinase



- Molecule 1: Pyrophosphate-dependent phosphofructokinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	211.90Å 89.32Å 115.46Å 90.00° 119.12° 90.00°	Depositor
Resolution (Å)	39.45 – 2.00 47.51 – 1.89	Depositor EDS
% Data completeness (in resolution range)	94.7 (39.45-2.00) 91.6 (47.51-1.89)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.57 (at 1.90Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.216 , 0.241 0.221 , 0.247	Depositor DCC
R_{free} test set	11281 reflections (4.16%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.610	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.8	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	0.94	EDS
Total number of atoms	12308	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: BR

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	0.33	0/3024	0.55	2/4090 (0.0%)
1	B	0.41	0/3024	0.60	3/4090 (0.1%)
1	C	0.33	0/3032	0.55	1/4100 (0.0%)
1	D	0.34	0/3028	0.56	1/4095 (0.0%)
All	All	0.35	0/12108	0.56	7/16375 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	GLY	C-N-CA	-6.45	108.75	122.30
1	B	273	GLY	N-CA-C	-5.98	98.16	113.10
1	B	272	GLY	C-N-CA	-5.93	109.85	122.30
1	A	34	GLY	N-CA-C	-5.90	98.34	113.10
1	D	34	GLY	N-CA-C	-5.82	98.54	113.10
1	C	273	GLY	N-CA-C	-5.53	99.27	113.10
1	B	34	GLY	N-CA-C	-5.46	99.45	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	A	2965	0	2931	67	0
1	B	2965	0	2931	62	0
1	C	2970	0	2940	78	0
1	D	2966	0	2937	75	0
2	C	1	0	0	0	0
3	A	94	0	0	0	0
3	B	130	0	0	1	0
3	C	89	0	0	2	0
3	D	128	0	0	5	0
All	All	12308	0	11739	282	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 12.

All (282) 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:C:255:LYS:HA	1:C:255:LYS:CE	1.49	1.35
1:C:255:LYS:CA	1:C:255:LYS:HE3	1.52	1.31
1:C:250:LYS:HB3	1:C:254:GLY:HA2	1.41	1.03
1:A:190:MET:H	1:A:299:GLN:HE22	1.19	0.90
1:B:358:ASN:O	1:B:359:VAL:HB	1.74	0.86
1:C:324:PHE:CD2	1:C:350[A]:MET:HE2	2.11	0.86
1:D:278:VAL:HA	1:D:281:MET:HE2	1.56	0.85
1:C:190:MET:H	1:C:299:GLN:HE22	1.23	0.85
1:C:255:LYS:HA	1:C:255:LYS:HE3	0.84	0.83
1:D:332:VAL:HG21	1:D:350[A]:MET:CE	2.08	0.83
1:D:190:MET:H	1:D:299:GLN:HE22	1.27	0.81
1:B:177:MET:HE3	1:B:177:MET:HA	1.63	0.81
1:B:190:MET:H	1:B:299:GLN:HE22	1.25	0.81
1:C:250:LYS:HD2	1:C:254:GLY:CA	2.10	0.81
1:B:177:MET:HA	1:B:177:MET:CE	2.13	0.79
1:D:143:VAL:O	1:D:197:ILE:HD11	1.82	0.79
1:D:406:LYS:HD3	3:D:510:HOH:O	1.80	0.79
1:A:250:LYS:CG	1:A:255:LYS:H	1.95	0.78
1:A:188:GLU:CD	1:A:274:VAL:HG12	2.06	0.77
1:C:255:LYS:HE3	1:C:255:LYS:C	2.05	0.76
1:C:255:LYS:O	1:C:256:PHE:CB	2.34	0.74
1:C:143:VAL:O	1:C:197:ILE:HD11	1.86	0.74
1:A:89:ASN:HD22	1:A:92:GLU:HB2	1.51	0.74
1:C:206:SER:HB3	1:C:207:PRO:HD2	1.69	0.73
1:B:90:ARG:O	1:B:94:GLU:HG3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:ALA:HB3	1:C:276:PRO:HD3	1.72	0.71
1:D:332:VAL:HG21	1:D:350[A]:MET:HE3	1.71	0.70
1:B:358:ASN:O	1:B:359:VAL:CB	2.38	0.70
1:A:159:VAL:HG11	1:A:197:ILE:HD12	1.73	0.70
1:D:332:VAL:HG21	1:D:350[A]:MET:HE2	1.73	0.70
1:D:283:LYS:HE3	1:D:290:TYR:CE2	2.27	0.69
1:A:250:LYS:CB	1:A:255:LYS:H	2.05	0.69
1:C:324:PHE:CG	1:C:350[A]:MET:CE	2.75	0.69
1:B:35:LYS:HD3	1:B:326:VAL:HG13	1.75	0.68
1:C:327:GLN:HG2	3:D:544:HOH:O	1.94	0.67
1:A:250:LYS:HG2	1:A:255:LYS:H	1.58	0.67
1:A:190:MET:H	1:A:299:GLN:NE2	1.90	0.66
1:C:255:LYS:CE	1:C:255:LYS:CA	2.35	0.66
1:D:357:ALA:O	1:D:359:VAL:HG23	1.96	0.66
1:A:188:GLU:OE1	1:A:274:VAL:HG12	1.95	0.65
1:D:124:SER:HB3	1:D:136:ALA:HB3	1.77	0.65
1:B:188:GLU:HB2	1:B:275:ALA:HB2	1.78	0.65
1:C:209:ARG:HH11	1:C:209:ARG:HG2	1.62	0.65
1:C:32:GLN:HG2	1:C:326:VAL:HG21	1.79	0.64
1:B:89:ASN:HD22	1:B:92:GLU:HB2	1.61	0.64
1:A:188:GLU:HG3	1:A:274:VAL:CG1	2.28	0.64
1:B:159:VAL:HG11	1:B:197:ILE:HD12	1.80	0.63
1:C:324:PHE:CG	1:C:350[A]:MET:HE2	2.32	0.63
1:D:15:THR:HG22	1:D:143:VAL:HG13	1.79	0.63
1:C:15:THR:HG22	1:C:143:VAL:HG13	1.81	0.62
1:A:250:LYS:HG2	1:A:255:LYS:N	2.15	0.62
1:B:206:SER:HB3	1:B:207:PRO:HD2	1.81	0.61
1:A:143:VAL:O	1:A:197:ILE:HD11	1.99	0.61
1:D:94:GLU:O	1:D:98:GLU:HG3	2.01	0.61
1:C:276:PRO:HG3	1:C:292:TRP:CZ2	2.35	0.61
1:D:384:ALA:HB3	1:D:385:PRO:HD3	1.82	0.61
1:D:206:SER:HB3	1:D:207:PRO:HD2	1.83	0.60
1:A:89:ASN:HD22	1:A:92:GLU:CB	2.13	0.60
1:D:209:ARG:HG2	1:D:209:ARG:HH11	1.67	0.60
1:C:126:LEU:O	1:C:130:LEU:HG	2.02	0.60
1:B:190:MET:H	1:B:299:GLN:NE2	1.97	0.59
1:D:190:MET:H	1:D:299:GLN:NE2	1.97	0.59
1:C:339:ILE:HD11	1:C:347:LYS:HG2	1.85	0.59
1:B:339:ILE:HD11	1:B:347:LYS:HE3	1.84	0.59
1:A:206:SER:HB3	1:A:207:PRO:HD2	1.85	0.59
1:C:32:GLN:HG3	1:C:35:LYS:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ASN:HB3	1:A:92:GLU:HB3	1.85	0.58
1:B:89:ASN:HD22	1:B:92:GLU:CB	2.16	0.58
1:B:356:VAL:O	1:B:357:ALA:C	2.39	0.58
1:B:305:ILE:HG13	1:B:305:ILE:O	2.04	0.58
1:C:190:MET:H	1:C:299:GLN:NE2	1.98	0.58
1:B:277:VAL:HG12	1:B:281:MET:HE3	1.86	0.58
1:D:275:ALA:HB3	1:D:276:PRO:HD3	1.86	0.58
1:A:250:LYS:HB3	1:A:254:GLY:HA2	1.85	0.57
1:C:254:GLY:O	1:C:255:LYS:HB2	2.04	0.57
1:A:358:ASN:OD1	1:A:359:VAL:N	2.38	0.57
1:B:94:GLU:O	1:B:98:GLU:HG3	2.04	0.57
1:D:32:GLN:HG2	1:D:326:VAL:HG21	1.85	0.57
1:D:190:MET:HE1	1:D:300:ARG:HB3	1.86	0.57
1:C:324:PHE:CD1	1:C:350[A]:MET:HE3	2.40	0.57
1:C:188:GLU:CD	1:C:274:VAL:HG12	2.26	0.56
1:D:278:VAL:HA	1:D:281:MET:CE	2.33	0.56
1:C:209:ARG:HG2	1:C:209:ARG:NH1	2.21	0.56
1:B:277:VAL:HG12	1:B:281:MET:CE	2.37	0.55
1:D:35:LYS:HD3	1:D:326:VAL:HG13	1.89	0.55
1:C:250:LYS:HD2	1:C:254:GLY:HA3	1.86	0.55
1:C:277:VAL:HG12	1:C:281:MET:HE3	1.87	0.55
1:D:2:ALA:HB3	1:D:104:ASP:OD1	2.07	0.55
1:B:143:VAL:O	1:B:197:ILE:HD11	2.06	0.55
1:B:159:VAL:CG1	1:B:197:ILE:HD12	2.36	0.55
1:C:35:LYS:HD3	1:C:326:VAL:HG13	1.88	0.55
1:B:148:PRO:HB3	1:B:359:VAL:HG12	1.89	0.54
1:A:339:ILE:HD11	1:A:347:LYS:HG2	1.88	0.54
1:D:90:ARG:O	1:D:94:GLU:HG3	2.06	0.54
1:A:356:VAL:O	1:A:358:ASN:O	2.26	0.54
1:B:276:PRO:HG3	1:B:292:TRP:CZ2	2.42	0.54
1:C:232:ASP:O	1:C:236:LYS:HG2	2.08	0.54
1:A:274:VAL:O	1:A:278:VAL:HG23	2.08	0.53
1:C:138:HIS:O	1:C:334:PRO:HD2	2.08	0.53
1:D:406:LYS:HE2	3:D:511:HOH:O	2.07	0.53
1:D:97:ILE:HG13	1:D:130:LEU:HD22	1.91	0.53
1:C:250:LYS:HD2	1:C:254:GLY:C	2.28	0.53
1:D:35:LYS:HE2	1:D:35:LYS:HA	1.91	0.53
1:D:209:ARG:HG2	1:D:209:ARG:NH1	2.23	0.53
1:B:89:ASN:HB3	1:B:92:GLU:HB3	1.91	0.53
1:B:275:ALA:HB3	1:B:276:PRO:HD3	1.90	0.53
1:A:52:GLU:O	1:A:52:GLU:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:VAL:HB	1:D:159:VAL:HG21	1.90	0.53
1:A:159:VAL:CG1	1:A:197:ILE:HD12	2.38	0.52
1:B:138:HIS:O	1:B:334:PRO:HD2	2.09	0.52
1:A:278:VAL:HA	1:A:281:MET:HE2	1.91	0.52
1:C:197:ILE:HG12	3:C:452:HOH:O	2.10	0.52
1:D:123:VAL:O	1:D:126:LEU:HB2	2.10	0.52
1:A:324:PHE:CZ	1:A:350:MET:HE2	2.45	0.52
1:C:218:PRO:HD2	1:C:219:GLU:OE1	2.09	0.52
1:C:194:ALA:HB1	1:C:196:TRP:CD1	2.45	0.52
1:D:406:LYS:HB2	1:D:406:LYS:NZ	2.25	0.51
1:A:278:VAL:HA	1:A:281:MET:CE	2.40	0.51
1:A:319:GLN:O	1:A:323:GLU:HG3	2.10	0.51
1:B:121:LEU:HD13	1:B:353:LEU:HB2	1.92	0.51
1:C:159:VAL:HG11	1:C:197:ILE:HD12	1.93	0.51
1:D:161:LYS:NZ	1:D:305:ILE:HD11	2.26	0.51
1:B:319:GLN:O	1:B:323:GLU:HG3	2.11	0.51
1:D:138:HIS:O	1:D:334:PRO:HD2	2.11	0.51
1:C:277:VAL:HG12	1:C:281:MET:CE	2.40	0.50
1:D:143:VAL:HG21	1:D:190:MET:HE3	1.94	0.50
1:D:91:ARG:HG3	3:D:423:HOH:O	2.10	0.50
1:B:32:GLN:O	1:B:33:SER:O	2.29	0.50
1:B:89:ASN:N	3:B:462:HOH:O	2.44	0.50
1:B:177:MET:CE	1:B:177:MET:CA	2.86	0.50
1:D:406:LYS:HE3	1:D:408:VAL:CG2	2.41	0.50
1:C:126:LEU:HB2	3:C:470:HOH:O	2.12	0.50
1:D:218:PRO:HD2	1:D:219:GLU:OE1	2.12	0.50
1:B:276:PRO:HG3	1:B:292:TRP:CH2	2.46	0.49
1:B:356:VAL:O	1:B:357:ALA:O	2.30	0.49
1:C:249:VAL:O	1:C:255:LYS:O	2.31	0.49
1:C:324:PHE:CE2	1:C:350[A]:MET:HE2	2.47	0.49
1:D:93:TYR:O	1:D:97:ILE:HG12	2.12	0.49
1:D:52:GLU:O	1:D:52:GLU:HG2	2.13	0.49
1:A:250:LYS:HD2	1:A:254:GLY:CA	2.43	0.49
1:B:161:LYS:NZ	1:B:305:ILE:HD11	2.28	0.49
1:C:143:VAL:HB	1:C:159:VAL:HG21	1.95	0.49
1:A:275:ALA:HB3	1:A:276:PRO:HD3	1.95	0.48
1:A:384:ALA:HB3	1:A:385:PRO:HD3	1.95	0.48
1:B:190:MET:HG3	1:B:299:GLN:CD	2.33	0.48
1:B:313:GLN:HB3	1:B:336:ILE:HD11	1.95	0.48
1:C:362:MET:SD	1:C:362:MET:N	2.82	0.48
1:D:159:VAL:HG11	1:D:197:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:GLU:HB2	1:D:275:ALA:HB2	1.95	0.48
1:A:188:GLU:HB2	1:A:275:ALA:HB2	1.94	0.48
1:B:127:SER:HB2	1:B:132:TYR:O	2.14	0.48
1:C:324:PHE:CG	1:C:350[A]:MET:HE3	2.48	0.48
1:A:147:LEU:HB2	1:A:153:CYS:SG	2.54	0.48
1:B:33:SER:HA	1:B:36:ILE:O	2.14	0.48
1:B:121:LEU:O	1:B:125:GLN:HG2	2.13	0.48
1:C:190:MET:HG3	1:C:299:GLN:CD	2.34	0.48
1:A:32:GLN:HG3	1:A:35:LYS:HB2	1.95	0.48
1:D:124:SER:CB	1:D:136:ALA:HB3	2.44	0.47
1:C:190:MET:HG3	1:C:299:GLN:OE1	2.14	0.47
1:D:49:ALA:O	1:D:99:VAL:HG21	2.14	0.47
1:D:283:LYS:HE3	1:D:290:TYR:HE2	1.77	0.47
1:A:138:HIS:O	1:A:334:PRO:HD2	2.14	0.47
1:C:33:SER:HA	1:C:36:ILE:O	2.15	0.47
1:D:276:PRO:HG3	1:D:292:TRP:CZ2	2.50	0.47
1:B:141:LYS:O	1:B:142:THR:HB	2.14	0.47
1:D:44:ASN:O	1:D:47:ILE:HG22	2.13	0.47
1:D:141:LYS:O	1:D:142:THR:HB	2.14	0.47
1:A:188:GLU:CG	1:A:274:VAL:CG1	2.93	0.47
1:A:276:PRO:HG3	1:A:292:TRP:CZ2	2.49	0.47
1:C:70:TYR:HB2	1:C:393:PRO:HB3	1.98	0.46
1:A:250:LYS:CG	1:A:255:LYS:N	2.69	0.46
1:A:250:LYS:HD2	1:A:254:GLY:HA2	1.98	0.46
1:D:370:GLU:CD	1:D:370:GLU:H	2.19	0.46
1:D:305:ILE:HG13	1:D:305:ILE:O	2.16	0.46
1:A:209:ARG:NH1	1:A:209:ARG:HG2	2.31	0.46
1:B:370:GLU:H	1:B:370:GLU:CD	2.19	0.46
1:C:43:ARG:O	1:C:44:ASN:HB2	2.16	0.46
1:C:90:ARG:O	1:C:94:GLU:HG3	2.15	0.46
1:B:52:GLU:O	1:B:52:GLU:HG2	2.16	0.46
1:B:93:TYR:HB3	1:B:126:LEU:HD23	1.97	0.46
1:C:8:TYR:O	1:C:41:ALA:HA	2.16	0.46
1:D:39:ILE:HB	1:D:57:THR:OG1	2.15	0.46
1:A:161:LYS:HE2	1:A:387:ILE:O	2.16	0.45
1:D:121:LEU:HD13	1:D:353:LEU:HB3	1.98	0.45
1:B:177:MET:HA	1:B:177:MET:HE2	1.95	0.45
1:D:406:LYS:HE3	1:D:408:VAL:HG23	1.97	0.45
1:A:222:PHE:HB3	1:A:251:GLY:HA2	1.97	0.45
1:C:384:ALA:HB3	1:C:385:PRO:HD3	1.98	0.45
1:D:339:ILE:HD11	1:D:347:LYS:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ILE:HG13	1:A:305:ILE:O	2.16	0.45
1:A:32:GLN:HB3	1:A:33:SER:H	1.62	0.45
1:B:93:TYR:O	1:B:97:ILE:HG12	2.16	0.45
1:B:384:ALA:HB3	1:B:385:PRO:HD3	1.98	0.45
1:C:165:VAL:O	1:C:169:GLU:HG3	2.16	0.45
1:A:141:LYS:O	1:A:142:THR:HB	2.16	0.45
1:C:253:ASP:O	1:C:254:GLY:O	2.35	0.45
1:D:32:GLN:CG	1:D:326:VAL:HG21	2.47	0.45
1:D:8:TYR:O	1:D:41:ALA:HA	2.16	0.44
1:C:138:HIS:CB	1:C:353:LEU:HD21	2.47	0.44
1:D:296:ASP:CG	1:D:297:TYR:H	2.18	0.44
1:C:188:GLU:HB2	1:C:275:ALA:HB2	1.98	0.44
1:D:21:SER:HB2	1:D:111:ASN:HD21	1.81	0.44
1:A:250:LYS:HB3	1:A:255:LYS:H	1.80	0.44
1:C:190:MET:HE1	1:C:300:ARG:HB3	2.00	0.44
1:C:255:LYS:HA	1:C:255:LYS:NZ	2.21	0.44
1:D:141:LYS:O	1:D:141:LYS:HE2	2.18	0.44
1:D:370:GLU:CD	1:D:370:GLU:N	2.71	0.44
1:A:324:PHE:CE1	1:A:350:MET:HE2	2.53	0.44
1:C:119:THR:O	1:C:123:VAL:HG23	2.18	0.44
1:A:33:SER:HA	1:A:36:ILE:O	2.18	0.44
1:C:35:LYS:HE2	1:C:35:LYS:HA	1.99	0.44
1:C:141:LYS:O	1:C:142:THR:HB	2.18	0.44
1:D:145:ASN:O	1:D:361:LYS:HE2	2.18	0.44
1:A:8:TYR:O	1:A:41:ALA:HA	2.18	0.43
1:B:89:ASN:ND2	1:B:92:GLU:N	2.66	0.43
1:B:148:PRO:CB	1:B:359:VAL:HG12	2.47	0.43
1:C:194:ALA:HB1	1:C:196:TRP:HD1	1.81	0.43
1:B:49:ALA:O	1:B:99:VAL:HG21	2.19	0.43
1:C:254:GLY:O	1:C:255:LYS:CB	2.64	0.43
1:D:147:LEU:HB2	1:D:153:CYS:SG	2.58	0.43
1:A:370:GLU:CD	1:A:370:GLU:H	2.21	0.43
1:B:89:ASN:ND2	1:B:92:GLU:H	2.15	0.43
1:C:305:ILE:HG13	1:C:305:ILE:O	2.19	0.43
1:D:254:GLY:O	1:D:255:LYS:HB3	2.18	0.43
1:D:324:PHE:CG	1:D:350[A]:MET:HE1	2.53	0.43
1:C:36:ILE:HG21	1:C:39:ILE:CD1	2.49	0.43
1:A:313:GLN:HB3	1:A:336:ILE:HD11	2.01	0.43
1:B:178:SER:HA	1:B:182:THR:O	2.18	0.43
1:C:72:PRO:HB3	1:C:303:ARG:HB2	2.01	0.43
1:B:112:GLY:O	1:B:138:HIS:HE1	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ARG:O	1:A:94:GLU:HG3	2.18	0.43
1:B:15:THR:HG22	1:B:143:VAL:HG13	2.00	0.43
1:B:50:LEU:HD21	1:B:92:GLU:HG3	2.01	0.42
1:B:90:ARG:HD2	1:B:94:GLU:OE2	2.19	0.42
1:C:188:GLU:OE1	1:C:274:VAL:HG12	2.19	0.42
1:D:33:SER:HA	1:D:36:ILE:O	2.19	0.42
1:A:21:SER:HB2	1:A:111:ASN:HD21	1.85	0.42
1:B:190:MET:HG3	1:B:299:GLN:OE1	2.18	0.42
1:A:208:GLU:HG3	1:A:209:ARG:HG3	2.00	0.42
1:D:161:LYS:O	1:D:165:VAL:HG23	2.20	0.42
1:A:32:GLN:O	1:A:33:SER:OG	2.35	0.42
1:C:147:LEU:HB2	1:C:153:CYS:SG	2.60	0.42
1:A:72:PRO:HB3	1:A:303:ARG:HB2	2.02	0.42
1:C:89:ASN:OD1	1:C:90:ARG:N	2.52	0.42
1:D:340:SER:HB3	1:D:345:GLN:OE1	2.19	0.42
1:B:8:TYR:O	1:B:41:ALA:HA	2.20	0.42
1:B:72:PRO:HB3	1:B:303:ARG:HB2	2.01	0.41
1:C:47:ILE:HD11	1:C:81:TYR:CD1	2.54	0.41
1:A:127:SER:HB2	1:A:132:TYR:O	2.20	0.41
1:A:305:ILE:O	1:A:305:ILE:HG23	2.20	0.41
1:C:7:PHE:HB2	1:C:105:ILE:HD13	2.02	0.41
1:D:80:ARG:C	3:D:454:HOH:O	2.59	0.41
1:D:161:LYS:HZ3	1:D:305:ILE:HD11	1.85	0.41
1:A:38:ARG:HG2	1:A:38:ARG:HH11	1.85	0.41
1:A:276:PRO:HG3	1:A:292:TRP:CH2	2.55	0.41
1:B:150:THR:O	1:B:361:LYS:HE3	2.20	0.41
1:B:370:GLU:CD	1:B:370:GLU:N	2.73	0.41
1:D:32:GLN:O	1:D:33:SER:C	2.59	0.41
1:A:250:LYS:HG2	1:A:255:LYS:CA	2.51	0.41
1:B:161:LYS:HD2	1:B:307:SER:HA	2.03	0.41
1:B:390:GLU:N	1:B:390:GLU:CD	2.74	0.41
1:D:148:PRO:HD3	1:D:359:VAL:O	2.21	0.41
1:A:209:ARG:HG2	1:A:209:ARG:HH11	1.85	0.41
1:A:250:LYS:HG2	1:A:255:LYS:HA	2.03	0.41
1:D:103:HIS:CE1	1:D:413:LYS:HD3	2.56	0.41
1:D:188:GLU:CD	1:D:274:VAL:HG12	2.41	0.41
1:D:276:PRO:HG3	1:D:292:TRP:CH2	2.56	0.41
1:A:254:GLY:O	1:A:255:LYS:CB	2.69	0.41
1:A:403:VAL:HG22	1:A:404:ARG:N	2.36	0.41
1:C:370:GLU:CD	1:C:370:GLU:H	2.24	0.41
1:A:188:GLU:CD	1:A:274:VAL:CG1	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:GLU:CD	1:A:370:GLU:N	2.74	0.40
1:C:29:ALA:HB1	1:C:39:ILE:HD11	2.02	0.40
1:D:232:ASP:O	1:D:236:LYS:HG2	2.21	0.40
1:C:21:SER:HB2	1:C:111:ASN:HD21	1.87	0.40
1:C:145:ASN:HB2	1:C:156:PHE:CG	2.56	0.40
1:C:273:GLY:O	1:C:277:VAL:HG23	2.22	0.40
1:D:81:TYR:HE2	1:D:92:GLU:OE1	2.04	0.40
1:A:143:VAL:HB	1:A:159:VAL:HG21	2.04	0.40
1:D:324:PHE:CD2	1:D:350[A]:MET:HE3	2.57	0.40
1:A:145:ASN:O	1:A:361:LYS:HE3	2.22	0.40
1:C:324:PHE:CD1	1:C:350[A]:MET:CE	3.03	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	387/419 (92%)	366 (95%)	17 (4%)	4 (1%)	15	9
1	B	387/419 (92%)	369 (95%)	12 (3%)	6 (2%)	9	4
1	C	388/419 (93%)	368 (95%)	16 (4%)	4 (1%)	15	9
1	D	387/419 (92%)	364 (94%)	19 (5%)	4 (1%)	15	9
All	All	1549/1676 (92%)	1467 (95%)	64 (4%)	18 (1%)	13	7

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	357	ALA
1	B	359	VAL
1	C	255	LYS
1	A	32	GLN

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Mol	Chain	Res	Type
1	A	33	SER
1	A	142	THR
1	B	33	SER
1	B	142	THR
1	C	142	THR
1	C	254	GLY
1	B	32	GLN
1	C	33	SER
1	D	32	GLN
1	D	142	THR
1	D	253	ASP
1	B	252	ASP
1	A	359	VAL
1	D	90	ARG

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	305/329 (93%)	299 (98%)	6 (2%)	55	58
1	B	305/329 (93%)	296 (97%)	9 (3%)	41	41
1	C	306/329 (93%)	300 (98%)	6 (2%)	55	58
1	D	306/329 (93%)	299 (98%)	7 (2%)	50	53
All	All	1222/1316 (93%)	1194 (98%)	28 (2%)	50	53

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	110	TYR
1	A	255	LYS
1	A	291	HIS
1	A	363	MET
1	A	370	GLU
1	B	32	GLN

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Mol	Chain	Res	Type
1	B	177	MET
1	B	255	LYS
1	B	284	GLU
1	B	358	ASN
1	B	359	VAL
1	B	361	LYS
1	B	370	GLU
1	B	404	ARG
1	C	47	ILE
1	C	129	THR
1	C	255	LYS
1	C	291	HIS
1	C	362	MET
1	C	370	GLU
1	D	32	GLN
1	D	91	ARG
1	D	104	ASP
1	D	130	LEU
1	D	225	GLN
1	D	370	GLU
1	D	406	LYS

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

Mol	Chain	Res	Type
1	A	89	ASN
1	A	111	ASN
1	A	125	GLN
1	A	138	HIS
1	A	299	GLN
1	B	89	ASN
1	B	125	GLN
1	B	138	HIS
1	B	291	HIS
1	B	299	GLN
1	C	111	ASN
1	C	135	GLN
1	C	138	HIS
1	C	291	HIS
1	C	299	GLN
1	C	319	GLN
1	D	89	ASN

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Mol	Chain	Res	Type
1	D	111	ASN
1	D	135	GLN
1	D	291	HIS
1	D	299	GLN
1	D	355	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	395/419 (94%)	0.12	25 (6%)	20 19	18, 29, 47, 55	0
1	B	395/419 (94%)	-0.05	13 (3%)	46 45	15, 25, 44, 54	0
1	C	395/419 (94%)	0.41	33 (8%)	11 10	17, 30, 48, 59	0
1	D	394/419 (94%)	0.06	20 (5%)	28 27	15, 27, 46, 58	0
All	All	1579/1676 (94%)	0.14	91 (5%)	23 22	15, 28, 46, 59	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	126	LEU	10.2
1	C	2	ALA	10.0
1	D	2	ALA	9.9
1	A	359	VAL	7.5
1	C	254	GLY	7.0
1	C	125	GLN	6.9
1	C	90	ARG	6.9
1	C	129	THR	6.5
1	C	253	ASP	6.1
1	C	3	ALA	6.1
1	C	89	ASN	5.9
1	D	3	ALA	5.8
1	D	130	LEU	5.8
1	C	128	GLY	5.1
1	D	358	ASN	5.0
1	D	125	GLN	4.9
1	A	362	MET	4.6
1	A	272	GLY	4.4
1	C	91	ARG	4.2
1	C	272	GLY	4.2
1	B	358	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	254	GLY	4.1
1	B	89	ASN	4.0
1	A	251	GLY	3.9
1	A	358	ASN	3.9
1	C	418	THR	3.6
1	A	252	ASP	3.6
1	D	128	GLY	3.5
1	C	131	GLY	3.4
1	D	253	ASP	3.4
1	A	225	GLN	3.2
1	B	357	ALA	3.2
1	A	255	LYS	3.2
1	C	255	LYS	3.2
1	D	92	GLU	3.2
1	B	272	GLY	3.1
1	D	225	GLN	3.1
1	D	33	SER	3.1
1	D	207	PRO	3.1
1	C	37	GLY	3.1
1	D	89	ASN	3.0
1	D	127	SER	3.0
1	A	370	GLU	2.9
1	A	256	PHE	2.8
1	A	207	PRO	2.8
1	C	209	ARG	2.8
1	D	284	GLU	2.8
1	B	418	THR	2.8
1	C	339	ILE	2.8
1	D	252	ASP	2.8
1	A	89	ASN	2.7
1	A	223	ASP	2.7
1	C	284	GLU	2.7
1	A	254	GLY	2.7
1	D	192	ARG	2.6
1	C	362	MET	2.5
1	C	358	ASN	2.5
1	A	253	ASP	2.5
1	B	90	ARG	2.5
1	A	339	ILE	2.4
1	A	92	GLU	2.4
1	C	340	SER	2.4
1	C	34	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	225	GLN	2.4
1	B	254	GLY	2.4
1	C	93	TYR	2.4
1	A	208	GLU	2.3
1	D	209	ARG	2.3
1	B	359	VAL	2.3
1	A	221	SER	2.3
1	C	365	GLU	2.3
1	C	343	PRO	2.3
1	C	251	GLY	2.3
1	C	370	GLU	2.3
1	A	284	GLU	2.3
1	A	165	VAL	2.2
1	B	92	GLU	2.2
1	B	208	GLU	2.2
1	C	301	ALA	2.2
1	D	339	ILE	2.1
1	A	34	GLY	2.1
1	C	127	SER	2.1
1	C	208	GLU	2.1
1	A	236	LYS	2.1
1	D	126	LEU	2.1
1	A	360	GLU	2.1
1	C	252	ASP	2.1
1	A	283	LYS	2.1
1	B	252	ASP	2.1
1	C	225	GLN	2.1
1	B	47	ILE	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BR	C	500	1/1	0.98	0.23	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.