Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:34 AM GMT

PDB ID	:	2HQA
Title	:	Crystal structure of the catalytic alpha subunit of E. Coli replicative DNA polymerase III
Authors	:	Lamers, M.H.; Georgescu, R.E.; Lee, S.G.; O'Donnell, M.; Kuriyan, J.
Deposited on	:	2006-07-18
Resolution	:	2.60 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:

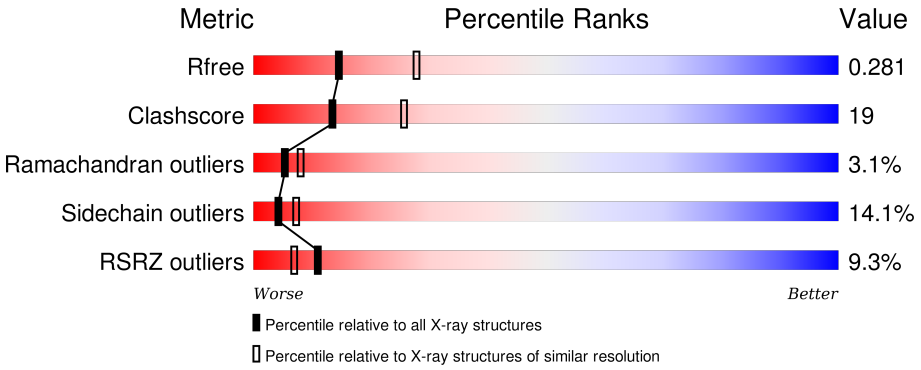
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	917	9% 63% 28% 8%

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
2	PO4	A	920	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7267 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 DNA polymerase III alpha subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	910	7148	4548	1219	1341	10	30	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	36	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	136	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	240	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	246	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	286	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	335	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	345	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	399	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	408	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	421	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	436	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	469	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	497	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	571	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	599	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	616	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	631	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	647	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	691	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	707	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	712	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	720	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	742	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	783	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	787	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	791	MSE	MET	MODIFIED RESIDUE	UNP P10443

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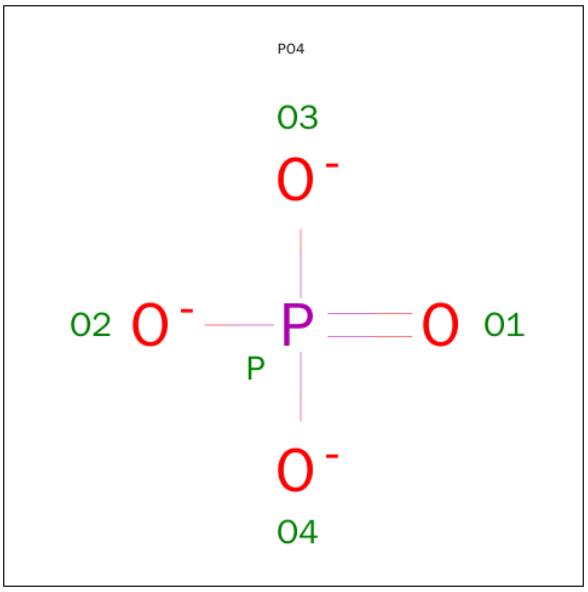
Chain	Residue	Modelled	Actual	Comment	Reference
A	807	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	884	MSE	MET	MODIFIED RESIDUE	UNP P10443
A	899	MSE	MET	MODIFIED RESIDUE	UNP P10443

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 3 is water.

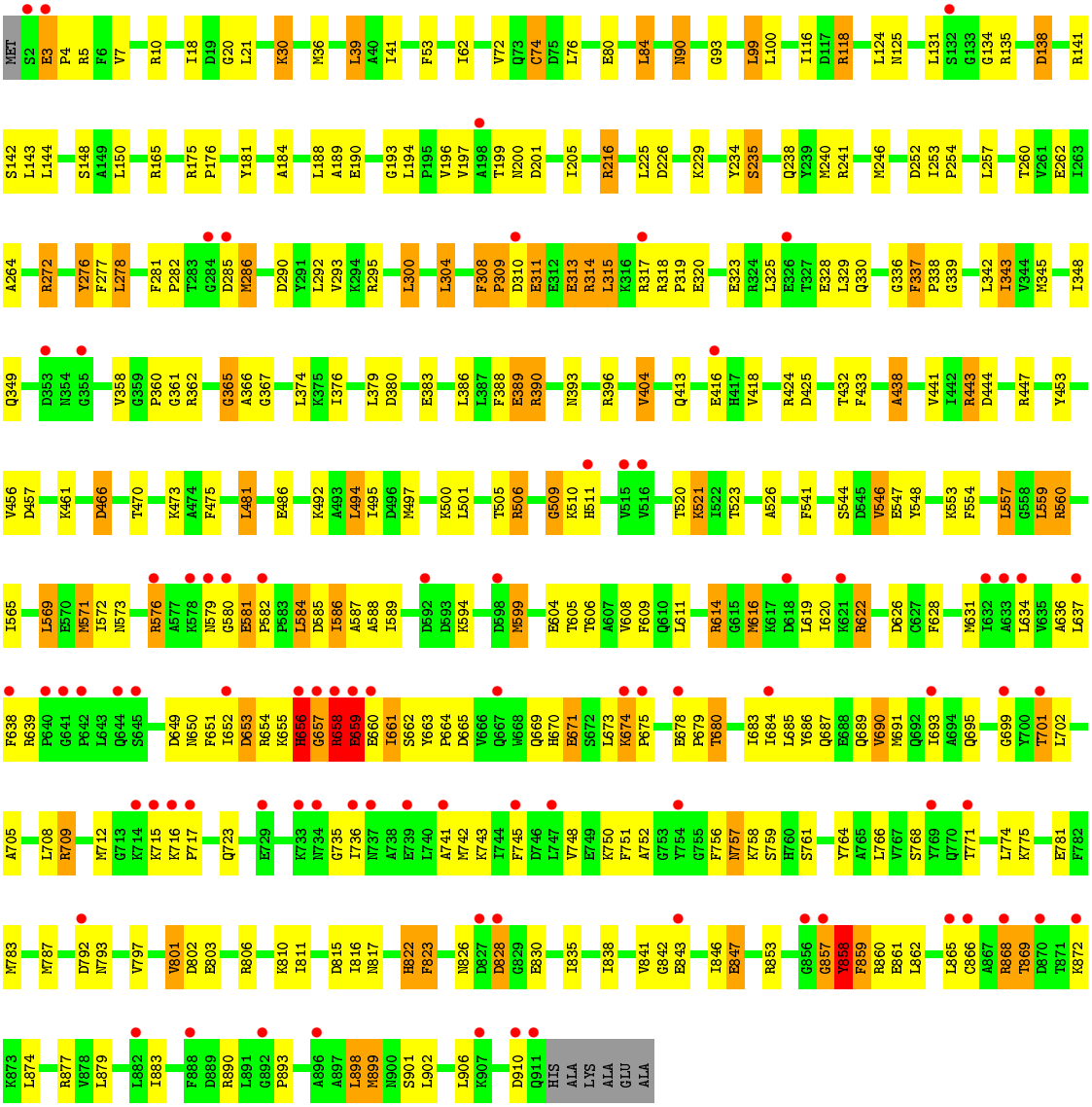
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	104	Total O 104 104	0	0

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: DNA polymerase III alpha subunit

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.11Å 98.26Å 139.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 19.91 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.7 (20.00-2.60) 96.7 (19.91-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.287 0.215 , 0.281	Depositor DCC
R_{free} test set	1736 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	68.2	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 69.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 34532 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7267	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: PO4

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	0.57	0/7269	0.68	4/9778 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	310	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	226	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	653	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	240	MSE	CG-SE-CE	-5.19	87.48	98.90

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	276	TYR	Peptide
1	A	308	PHE	Peptide
1	A	509	GLY	Peptide
1	A	656	HIS	Peptide
1	A	657	GLY	Peptide
1	A	658	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	A	659	GLU	Peptide
1	A	857	GLY	Peptide
1	A	858	TYR	Peptide

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	7148	0	7086	266	1
2	A	15	0	0	3	0
3	A	104	0	0	1	0
All	All	7267	0	7086	266	1

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 19.

All (266) 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:A:656:HIS:HB2	1:A:657:GLY:HA2	1.17	1.13
1:A:659:GLU:HG2	1:A:660:GLU:H	1.08	1.10
1:A:7:VAL:H	1:A:260:THR:HG21	1.19	1.08
1:A:659:GLU:CG	1:A:660:GLU:H	1.68	1.04
1:A:822:HIS:O	1:A:823:PHE:HB2	1.56	1.02
1:A:241:ARG:HB2	1:A:246:MSE:HE1	1.43	1.00
1:A:659:GLU:HG2	1:A:660:GLU:N	1.59	0.99
1:A:768:SER:O	1:A:771:THR:HG22	1.63	0.98
1:A:509:GLY:CA	1:A:510:LYS:HB3	1.95	0.96
1:A:826:ASN:HD22	1:A:830:GLU:HB2	1.27	0.96
1:A:7:VAL:H	1:A:260:THR:CG2	1.79	0.96
1:A:339:GLY:O	1:A:343:ILE:HG22	1.67	0.94
1:A:241:ARG:CB	1:A:246:MSE:HE1	1.99	0.93
1:A:509:GLY:HA2	1:A:510:LYS:HB3	1.49	0.93
1:A:879:LEU:O	1:A:883:ILE:HG12	1.69	0.92
1:A:690:VAL:HG21	1:A:752:ALA:HB2	1.51	0.92
1:A:3:GLU:HB3	1:A:4:PRO:HD3	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ARG:HG2	1:A:118:ARG:HH11	1.35	0.91
1:A:443:ARG:HH11	1:A:443:ARG:HG2	1.38	0.89
1:A:3:GLU:HB3	1:A:4:PRO:CD	2.02	0.88
1:A:663:TYR:H	1:A:669:GLN:HG3	1.38	0.88
1:A:509:GLY:HA2	1:A:510:LYS:CB	2.05	0.86
1:A:656:HIS:CB	1:A:657:GLY:HA2	2.04	0.86
1:A:586:ILE:O	1:A:589:ILE:HG12	1.77	0.84
1:A:585:ASP:OD2	1:A:587:ALA:HB3	1.77	0.84
1:A:257:LEU:O	1:A:260:THR:HB	1.79	0.83
1:A:858:TYR:CZ	1:A:868:ARG:HG3	2.13	0.83
1:A:653:ASP:O	1:A:657:GLY:HA3	1.79	0.82
1:A:858:TYR:OH	1:A:868:ARG:HG3	1.78	0.82
1:A:626:ASP:OD2	1:A:655:LYS:NZ	2.13	0.82
1:A:656:HIS:HB2	1:A:657:GLY:CA	2.07	0.79
1:A:118:ARG:HH11	1:A:118:ARG:CG	1.96	0.78
1:A:580:GLY:HA2	1:A:581:GLU:O	1.84	0.77
1:A:7:VAL:N	1:A:260:THR:HG21	1.99	0.76
1:A:787:MSE:HE1	1:A:801:VAL:HG12	1.66	0.75
1:A:608:VAL:HB	1:A:771:THR:HG23	1.68	0.74
1:A:783:MSE:O	1:A:787:MSE:HG3	1.86	0.74
1:A:300:LEU:HD22	1:A:304:LEU:HD22	1.70	0.73
1:A:241:ARG:CB	1:A:246:MSE:CE	2.67	0.71
1:A:313:GLU:HG3	1:A:314:ARG:H	1.54	0.71
1:A:235:SER:H	1:A:238:GLN:HE21	1.39	0.71
1:A:241:ARG:HB3	1:A:246:MSE:CE	2.22	0.70
1:A:339:GLY:O	1:A:343:ILE:CG2	2.39	0.70
1:A:118:ARG:HG2	1:A:118:ARG:NH1	2.08	0.69
1:A:659:GLU:CG	1:A:660:GLU:N	2.33	0.69
1:A:557:LEU:HD13	1:A:559:LEU:HD23	1.73	0.69
1:A:315:LEU:H	1:A:315:LEU:HD12	1.58	0.69
1:A:674:LYS:CB	1:A:675:PRO:HD3	2.24	0.68
1:A:841:VAL:HG23	1:A:842:GLY:H	1.59	0.68
1:A:389:GLU:HG3	1:A:702:LEU:HB3	1.76	0.68
1:A:674:LYS:O	1:A:678:GLU:HG2	1.93	0.67
1:A:318:ARG:N	1:A:319:PRO:HD2	2.09	0.66
1:A:285:ASP:O	1:A:286:MSE:HB2	1.94	0.66
1:A:608:VAL:HG23	1:A:611:LEU:CD1	2.26	0.65
1:A:286:MSE:HE2	1:A:290:ASP:HB3	1.79	0.65
1:A:131:LEU:HD22	1:A:197:VAL:HG11	1.78	0.65
1:A:509:GLY:HA3	1:A:510:LYS:HB3	1.78	0.65
1:A:653:ASP:HB3	1:A:658:ARG:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:ASP:O	1:A:587:ALA:N	2.30	0.65
1:A:631:MSE:HA	1:A:634:LEU:HD12	1.78	0.64
1:A:693:ILE:HD11	1:A:748:VAL:HG21	1.78	0.64
1:A:650:ASN:O	1:A:654:ARG:HB2	1.97	0.64
1:A:39:LEU:O	1:A:53:PHE:HZ	1.79	0.64
1:A:390:ARG:CG	1:A:691:MSE:HE1	2.28	0.64
1:A:199:THR:HG22	1:A:201:ASP:H	1.62	0.64
1:A:866:CYS:HA	1:A:869:THR:HG22	1.80	0.63
1:A:457:ASP:OD2	1:A:461:LYS:HE3	1.98	0.63
1:A:300:LEU:HD12	1:A:325:LEU:HD22	1.81	0.63
1:A:572:ILE:HG21	1:A:584:LEU:HD12	1.81	0.63
1:A:404:VAL:HG12	1:A:554:PHE:CD2	2.33	0.62
1:A:684:ILE:HD13	1:A:748:VAL:HG23	1.80	0.62
1:A:585:ASP:C	1:A:587:ALA:H	2.03	0.62
1:A:858:TYR:OH	1:A:868:ARG:CG	2.47	0.62
1:A:7:VAL:HG22	1:A:260:THR:CG2	2.30	0.62
1:A:199:THR:CG2	1:A:201:ASP:H	2.12	0.62
1:A:652:ILE:HG13	1:A:653:ASP:N	2.15	0.61
1:A:559:LEU:HD13	1:A:560:ARG:NH2	2.15	0.61
1:A:10:ARG:HB3	1:A:199:THR:CG2	2.30	0.61
1:A:313:GLU:O	1:A:315:LEU:N	2.33	0.61
1:A:810:LYS:HB2	1:A:830:GLU:HG2	1.83	0.61
1:A:3:GLU:CB	1:A:4:PRO:HD3	2.29	0.60
1:A:585:ASP:OD2	1:A:587:ALA:CB	2.49	0.60
1:A:10:ARG:HB3	1:A:199:THR:HG23	1.84	0.60
1:A:683:ILE:HG23	1:A:751:PHE:HE2	1.66	0.59
1:A:7:VAL:HG22	1:A:260:THR:HG23	1.85	0.59
1:A:826:ASN:HB2	1:A:830:GLU:H	1.67	0.59
1:A:745:PHE:HA	1:A:748:VAL:HG12	1.84	0.59
1:A:674:LYS:HB2	1:A:675:PRO:HD3	1.85	0.58
1:A:544:SER:O	1:A:547:GLU:HB3	2.02	0.58
1:A:573:ASN:O	1:A:576:ARG:HB3	2.04	0.57
1:A:90:ASN:HD22	1:A:90:ASN:C	2.08	0.57
1:A:670:HIS:HB3	1:A:673:LEU:HD13	1.86	0.57
1:A:390:ARG:HG3	1:A:691:MSE:HE1	1.87	0.57
1:A:822:HIS:O	1:A:823:PHE:CB	2.39	0.56
1:A:608:VAL:HG23	1:A:611:LEU:HD12	1.87	0.56
1:A:619:LEU:HA	1:A:622:ARG:HB3	1.88	0.56
1:A:585:ASP:C	1:A:587:ALA:N	2.55	0.55
1:A:443:ARG:HH11	1:A:443:ARG:CG	2.17	0.55
1:A:802:ASP:O	1:A:806:ARG:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:GLY:HA2	1:A:181:TYR:CE2	2.42	0.55
1:A:655:LYS:HG2	1:A:656:HIS:H	1.72	0.54
1:A:343:ILE:O	1:A:343:ILE:HG12	2.06	0.54
1:A:817:ASN:OD1	1:A:859:PHE:HB2	2.07	0.54
1:A:605:THR:HG21	1:A:620:ILE:HD13	1.89	0.54
1:A:390:ARG:HG2	1:A:691:MSE:HE1	1.89	0.54
1:A:444:ASP:OD2	1:A:506:ARG:NH2	2.41	0.54
1:A:36:MSE:O	1:A:62:ILE:HD12	2.08	0.54
1:A:609:PHE:H	1:A:771:THR:HG21	1.73	0.54
1:A:125:ASN:O	1:A:165:ARG:NH2	2.41	0.54
1:A:315:LEU:H	1:A:315:LEU:CD1	2.21	0.53
1:A:678:GLU:N	1:A:679:PRO:HD2	2.24	0.53
1:A:559:LEU:HD13	1:A:560:ARG:HH22	1.74	0.53
1:A:379:LEU:HG	1:A:766:LEU:HD22	1.90	0.53
1:A:841:VAL:HG23	1:A:842:GLY:N	2.24	0.53
1:A:606:THR:HG21	1:A:803:GLU:HG3	1.91	0.53
1:A:393:ASN:HB3	1:A:396:ARG:HG2	1.90	0.53
1:A:893:PRO:HB2	1:A:898:LEU:HD22	1.91	0.52
1:A:470:THR:HG23	1:A:473:LYS:H	1.75	0.52
1:A:235:SER:H	1:A:238:GLN:NE2	2.05	0.52
1:A:701:THR:O	1:A:702:LEU:HB2	2.10	0.52
1:A:234:TYR:HA	1:A:238:GLN:HE22	1.74	0.52
1:A:444:ASP:OD1	1:A:447:ARG:NH2	2.43	0.52
1:A:100:LEU:HD22	1:A:116:ILE:HG21	1.91	0.52
1:A:690:VAL:HG21	1:A:752:ALA:CB	2.32	0.51
1:A:816:ILE:O	1:A:853:ARG:NH1	2.42	0.51
1:A:565:ILE:O	1:A:569:LEU:HB2	2.10	0.51
1:A:838:ILE:O	1:A:841:VAL:HG22	2.10	0.51
1:A:216:ARG:NH2	1:A:505:THR:O	2.44	0.51
1:A:390:ARG:CZ	1:A:709:ARG:HH12	2.23	0.51
1:A:453:TYR:O	1:A:456:VAL:HG12	2.10	0.50
1:A:571:MSE:HG2	1:A:781:GLU:HG3	1.94	0.50
1:A:7:VAL:HA	1:A:36:MSE:HE3	1.93	0.50
1:A:756:PHE:HD1	1:A:761:SER:HB2	1.76	0.50
1:A:365:GLY:C	1:A:367:GLY:H	2.14	0.50
1:A:475:PHE:CE1	1:A:481:LEU:HG	2.47	0.50
1:A:655:LYS:CG	1:A:656:HIS:N	2.75	0.50
1:A:614:ARG:H	1:A:614:ARG:HD3	1.76	0.49
1:A:683:ILE:HG23	1:A:751:PHE:CE2	2.45	0.49
1:A:308:PHE:O	1:A:309:PRO:O	2.30	0.49
1:A:380:ASP:OD2	1:A:383:GLU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:PHE:CD2	1:A:683:ILE:HD13	2.48	0.49
1:A:899:MSE:CE	1:A:899:MSE:HA	2.42	0.49
1:A:365:GLY:O	1:A:759:SER:OG	2.31	0.49
1:A:319:PRO:O	1:A:323:GLU:HB2	2.13	0.49
1:A:693:ILE:HD11	1:A:748:VAL:CG2	2.43	0.48
1:A:756:PHE:CD1	1:A:761:SER:HB2	2.48	0.48
1:A:199:THR:CG2	1:A:200:ASN:N	2.75	0.48
1:A:497:MSE:HB2	1:A:497:MSE:HE2	1.71	0.48
1:A:72:VAL:HG11	1:A:84:LEU:HB2	1.96	0.48
1:A:757:ASN:C	1:A:757:ASN:HD22	2.16	0.48
1:A:797:VAL:O	1:A:801:VAL:HG13	2.13	0.48
1:A:432:THR:HA	2:A:920:PO4:O2	2.13	0.48
1:A:686:TYR:CE2	1:A:758:LYS:HE3	2.49	0.48
1:A:254:PRO:HA	1:A:257:LEU:HD12	1.96	0.48
1:A:241:ARG:HB3	1:A:246:MSE:HE2	1.95	0.48
1:A:669:GLN:HG2	1:A:670:HIS:N	2.28	0.48
1:A:10:ARG:HG2	1:A:201:ASP:HA	1.95	0.48
1:A:486:GLU:OE1	1:A:486:GLU:HA	2.13	0.48
1:A:345:MSE:HB2	1:A:374:LEU:HD13	1.96	0.47
1:A:272:ARG:NH2	1:A:277:PHE:CZ	2.82	0.47
1:A:30:LYS:HG3	1:A:205:ILE:HG23	1.96	0.47
1:A:125:ASN:HD21	1:A:165:ARG:HH12	1.61	0.47
1:A:708:LEU:O	1:A:712:MSE:HG3	2.14	0.47
1:A:281:PHE:CG	1:A:282:PRO:HD2	2.49	0.47
1:A:637:LEU:O	1:A:639:ARG:N	2.46	0.47
1:A:835:ILE:HG23	1:A:838:ILE:HD12	1.97	0.47
1:A:292:LEU:HD22	1:A:338:PRO:HA	1.96	0.47
1:A:74:CYS:SG	1:A:76:LEU:HB2	2.55	0.47
1:A:241:ARG:HB2	1:A:246:MSE:CE	2.26	0.47
1:A:199:THR:HG22	1:A:201:ASP:N	2.29	0.47
1:A:599:MSE:HE3	1:A:604:GLU:HB2	1.96	0.47
1:A:826:ASN:HB3	1:A:828:ASP:H	1.80	0.47
1:A:687:GLN:O	1:A:690:VAL:HG12	2.14	0.47
1:A:655:LYS:HG2	1:A:656:HIS:N	2.30	0.47
1:A:608:VAL:HG23	1:A:611:LEU:HD11	1.97	0.47
1:A:671:GLU:O	1:A:674:LYS:HG3	2.15	0.46
1:A:510:LYS:HG2	1:A:511:HIS:N	2.29	0.46
1:A:690:VAL:CG2	1:A:748:VAL:HG22	2.46	0.46
1:A:201:ASP:OD2	2:A:918:PO4:O4	2.33	0.46
1:A:686:TYR:HB2	1:A:689:GLN:HG3	1.97	0.46
1:A:674:LYS:CB	1:A:675:PRO:CD	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ASN:ND2	1:A:93:GLY:H	2.14	0.46
1:A:735:GLY:HA2	1:A:736:ILE:HA	1.56	0.46
1:A:702:LEU:HA	1:A:705:ALA:HB3	1.98	0.46
1:A:608:VAL:HB	1:A:771:THR:CG2	2.43	0.46
1:A:605:THR:HB	1:A:608:VAL:HG22	1.98	0.46
1:A:336:GLY:C	1:A:338:PRO:HD2	2.36	0.46
1:A:557:LEU:HD23	1:A:557:LEU:HA	1.85	0.46
1:A:90:ASN:HD22	1:A:93:GLY:H	1.63	0.46
1:A:313:GLU:CG	1:A:314:ARG:H	2.28	0.46
1:A:235:SER:N	1:A:238:GLN:HE21	2.09	0.45
1:A:337:PHE:N	1:A:338:PRO:CD	2.80	0.45
1:A:659:GLU:HG3	1:A:660:GLU:H	1.73	0.45
1:A:857:GLY:O	1:A:858:TYR:HB2	2.15	0.45
1:A:365:GLY:O	1:A:366:ALA:HB3	2.16	0.45
1:A:7:VAL:HG21	1:A:264:ALA:HB2	1.97	0.45
1:A:576:ARG:HG3	1:A:581:GLU:O	2.16	0.45
1:A:609:PHE:HE1	1:A:764:TYR:HD2	1.65	0.45
1:A:628:PHE:O	1:A:631:MSE:HB2	2.16	0.45
1:A:189:ALA:HB1	1:A:194:LEU:O	2.17	0.45
1:A:872:LYS:HD3	1:A:872:LYS:HA	1.75	0.45
1:A:787:MSE:CE	1:A:801:VAL:HG12	2.39	0.45
1:A:317:ARG:HE	1:A:320:GLU:CD	2.20	0.45
1:A:683:ILE:HD12	1:A:683:ILE:H	1.81	0.45
1:A:328:GLU:OE1	1:A:388:PHE:HB2	2.17	0.44
1:A:716:LYS:HG2	1:A:717:PRO:HD2	1.99	0.44
1:A:520:THR:O	1:A:521:LYS:C	2.54	0.44
1:A:541:PHE:HA	3:A:984:HOH:O	2.16	0.44
1:A:348:ILE:HD12	1:A:376:ILE:HG23	1.99	0.44
1:A:118:ARG:NH1	1:A:118:ARG:CG	2.68	0.44
1:A:216:ARG:HB2	1:A:501:LEU:HD11	1.99	0.44
1:A:616:MSE:HE1	1:A:634:LEU:HB3	2.00	0.44
1:A:661:ILE:HG13	1:A:661:ILE:H	1.57	0.44
1:A:390:ARG:NH2	1:A:709:ARG:HH12	2.16	0.44
1:A:10:ARG:HB3	1:A:199:THR:HG21	1.99	0.44
1:A:695:GLN:O	1:A:699:GLY:HA2	2.17	0.44
1:A:313:GLU:HG3	1:A:314:ARG:N	2.29	0.44
1:A:546:VAL:CG1	1:A:547:GLU:N	2.82	0.43
1:A:622:ARG:HG3	1:A:622:ARG:O	2.18	0.43
1:A:276:TYR:HB3	1:A:278:LEU:HD13	2.01	0.43
1:A:781:GLU:OE2	1:A:781:GLU:N	2.52	0.43
1:A:466:ASP:N	1:A:466:ASP:OD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:TYR:HA	1:A:238:GLN:NE2	2.34	0.43
1:A:651:PHE:HD2	1:A:683:ILE:HD13	1.82	0.43
1:A:599:MSE:HE1	1:A:604:GLU:O	2.19	0.43
1:A:143:LEU:HD22	1:A:184:ALA:HB1	2.01	0.43
1:A:686:TYR:CG	1:A:758:LYS:HB2	2.54	0.43
1:A:657:GLY:O	1:A:658:ARG:O	2.36	0.43
1:A:20:GLY:O	1:A:216:ARG:HD2	2.19	0.42
1:A:680:THR:HG22	1:A:689:GLN:HE22	1.84	0.42
1:A:285:ASP:O	1:A:286:MSE:CB	2.64	0.42
1:A:547:GLU:OE1	1:A:547:GLU:HA	2.18	0.42
1:A:741:ALA:C	1:A:743:LYS:H	2.22	0.42
1:A:658:ARG:HB3	1:A:659:GLU:H	1.77	0.42
1:A:571:MSE:HE3	1:A:781:GLU:O	2.19	0.42
1:A:135:ARG:NH1	1:A:176:PRO:O	2.52	0.42
1:A:7:VAL:CG2	1:A:260:THR:HG23	2.48	0.42
1:A:39:LEU:O	1:A:53:PHE:CZ	2.67	0.42
1:A:475:PHE:HZ	1:A:495:ILE:HD13	1.84	0.42
1:A:636:ALA:O	1:A:639:ARG:HD3	2.20	0.42
1:A:433:PHE:N	2:A:920:PO4:O2	2.48	0.41
1:A:438:ALA:O	1:A:441:VAL:HG12	2.20	0.41
1:A:581:GLU:HA	1:A:582:PRO:HD2	1.90	0.41
1:A:41:ILE:HD12	1:A:53:PHE:CE1	2.55	0.41
1:A:367:GLY:HA2	1:A:386:LEU:HB3	2.01	0.41
1:A:680:THR:OG1	1:A:680:THR:O	2.37	0.41
1:A:546:VAL:HG12	1:A:547:GLU:N	2.36	0.41
1:A:199:THR:HG22	1:A:200:ASN:N	2.35	0.41
1:A:846:ILE:O	1:A:847:GLU:C	2.59	0.41
1:A:586:ILE:C	1:A:589:ILE:HG12	2.38	0.41
1:A:843:GLU:O	1:A:847:GLU:HB2	2.20	0.41
1:A:815:ASP:HB2	1:A:890:ARG:NH1	2.36	0.41
1:A:768:SER:C	1:A:771:THR:HG22	2.36	0.41
1:A:189:ALA:O	1:A:193:GLY:N	2.53	0.41
1:A:605:THR:HB	1:A:608:VAL:CG2	2.51	0.40
1:A:389:GLU:OE2	1:A:389:GLU:N	2.54	0.40
1:A:680:THR:CG2	1:A:689:GLN:HE22	2.34	0.40
1:A:313:GLU:O	1:A:314:ARG:C	2.59	0.40
1:A:99:LEU:HD12	1:A:99:LEU:HA	1.78	0.40
1:A:663:TYR:O	1:A:673:LEU:HD22	2.21	0.40
1:A:311:GLU:HG3	1:A:313:GLU:HG2	2.03	0.40
1:A:585:ASP:O	1:A:588:ALA:N	2.45	0.40
1:A:599:MSE:HE1	1:A:775:LYS:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:THR:HA	1:A:526:ALA:O	2.22	0.40
1:A:858:TYR:O	1:A:859:PHE:CB	2.70	0.40
1:A:416:GLU:HA	1:A:416:GLU:OE1	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:GLU:OE2	1:A:877:ARG:NH2[4_565]	2.08	0.12

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	908/917 (99%)	798 (88%)	82 (9%)	28 (3%)	5 8

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	PRO
1	A	314	ARG
1	A	658	ARG
1	A	859	PHE
1	A	315	LEU
1	A	361	GLY
1	A	521	LYS
1	A	910	ASP
1	A	360	PRO
1	A	494	LEU
1	A	638	PHE
1	A	858	TYR
1	A	138	ASP

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Mol	Chain	Res	Type
1	A	362	ARG
1	A	579	ASN
1	A	581	GLU
1	A	664	PRO
1	A	674	LYS
1	A	715	LYS
1	A	742	MSE
1	A	823	PHE
1	A	286	MSE
1	A	424	ARG
1	A	438	ALA
1	A	365	GLY
1	A	337	PHE
1	A	3	GLU
1	A	586	ILE

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	753/727 (104%)	647 (86%)	106 (14%)	4 7

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	18	ILE
1	A	21	LEU
1	A	30	LYS
1	A	39	LEU
1	A	74	CYS
1	A	80	GLU
1	A	84	LEU
1	A	90	ASN
1	A	99	LEU
1	A	118	ARG

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Mol	Chain	Res	Type
1	A	124	LEU
1	A	138	ASP
1	A	141	ARG
1	A	142	SER
1	A	144	LEU
1	A	148	SER
1	A	150	LEU
1	A	175	ARG
1	A	188	LEU
1	A	196	VAL
1	A	216	ARG
1	A	225	LEU
1	A	229	LYS
1	A	235	SER
1	A	252	ASP
1	A	253	ILE
1	A	262	GLU
1	A	272	ARG
1	A	278	LEU
1	A	293	VAL
1	A	295	ARG
1	A	300	LEU
1	A	304	LEU
1	A	311	GLU
1	A	313	GLU
1	A	329	LEU
1	A	330	GLN
1	A	342	LEU
1	A	343	ILE
1	A	349	GLN
1	A	358	VAL
1	A	389	GLU
1	A	390	ARG
1	A	404	VAL
1	A	413	GLN
1	A	418	VAL
1	A	425	ASP
1	A	443	ARG
1	A	466	ASP
1	A	481	LEU
1	A	492	LYS
1	A	494	LEU

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Mol	Chain	Res	Type
1	A	500	LYS
1	A	506	ARG
1	A	546	VAL
1	A	548	TYR
1	A	553	LYS
1	A	557	LEU
1	A	559	LEU
1	A	560	ARG
1	A	569	LEU
1	A	571	MSE
1	A	576	ARG
1	A	584	LEU
1	A	594	LYS
1	A	599	MSE
1	A	614	ARG
1	A	616	MSE
1	A	622	ARG
1	A	649	ASP
1	A	656	HIS
1	A	659	GLU
1	A	661	ILE
1	A	662	SER
1	A	665	ASP
1	A	671	GLU
1	A	680	THR
1	A	685	LEU
1	A	690	VAL
1	A	701	THR
1	A	709	ARG
1	A	723	GLN
1	A	750	LYS
1	A	757	ASN
1	A	774	LEU
1	A	792	ASP
1	A	793	ASN
1	A	801	VAL
1	A	811	ILE
1	A	822	HIS
1	A	828	ASP
1	A	847	GLU
1	A	858	TYR
1	A	860	ARG

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Mol	Chain	Res	Type
1	A	861	GLU
1	A	862	LEU
1	A	865	LEU
1	A	868	ARG
1	A	869	THR
1	A	874	LEU
1	A	898	LEU
1	A	899	MSE
1	A	901	SER
1	A	902	LEU
1	A	906	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	125	ASN
1	A	220	HIS
1	A	238	GLN
1	A	349	GLN
1	A	601	GLN
1	A	669	GLN
1	A	670	HIS
1	A	692	GLN
1	A	757	ASN
1	A	793	ASN
1	A	826	ASN
1	A	854	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

3 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	PO4	A	918	-	4,4,4	0.44	0	6,6,6	0.27	0
2	PO4	A	919	-	4,4,4	0.37	0	6,6,6	0.28	0
2	PO4	A	920	-	4,4,4	0.43	0	6,6,6	0.26	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	918	-	-	0/0/0/0	0/0/0/0
2	PO4	A	919	-	-	0/0/0/0	0/0/0/0
2	PO4	A	920	-	-	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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	918	PO4	1	0
2	A	920	PO4	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	880/917 (95%)	0.53	82 (9%)	11	7	35, 65, 73, 86	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	310	ASP	7.2
1	A	911	GLN	4.8
1	A	579	ASN	4.8
1	A	872	LYS	4.8
1	A	634	LEU	4.7
1	A	645	SER	4.7
1	A	736	ILE	4.6
1	A	580	GLY	4.6
1	A	656	HIS	4.6
1	A	857	GLY	4.5
1	A	868	ARG	3.8
1	A	644	GLN	3.8
1	A	633	ALA	3.7
1	A	657	GLY	3.6
1	A	2	SER	3.6
1	A	659	GLU	3.6
1	A	739	GLU	3.6
1	A	737	ASN	3.6
1	A	716	LYS	3.5
1	A	827	ASP	3.5
1	A	621	LYS	3.5
1	A	674	LYS	3.5
1	A	747	LEU	3.4
1	A	717	PRO	3.4
1	A	632	ILE	3.3
1	A	734	ASN	3.2
1	A	699	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	675	PRO	3.1
1	A	582	PRO	3.1
1	A	641	GLY	3.0
1	A	714	LYS	3.0
1	A	771	THR	3.0
1	A	910	ASP	2.9
1	A	637	LEU	2.9
1	A	618	ASP	2.8
1	A	598	ASP	2.8
1	A	578	LYS	2.8
1	A	769	TYR	2.8
1	A	660	GLU	2.7
1	A	355	GLY	2.6
1	A	516	VAL	2.6
1	A	888	PHE	2.6
1	A	640	PRO	2.5
1	A	856	GLY	2.5
1	A	317	ARG	2.5
1	A	907	LYS	2.5
1	A	667	GLN	2.5
1	A	353	ASP	2.5
1	A	733	LYS	2.4
1	A	326	GLU	2.4
1	A	729	GLU	2.4
1	A	652	ILE	2.4
1	A	896	ALA	2.4
1	A	132	SER	2.4
1	A	865	LEU	2.3
1	A	198	ALA	2.3
1	A	592	ASP	2.3
1	A	416	GLU	2.3
1	A	754	TYR	2.3
1	A	576	ARG	2.3
1	A	642	PRO	2.3
1	A	866	CYS	2.3
1	A	285	ASP	2.3
1	A	843	GLU	2.2
1	A	828	ASP	2.2
1	A	678	GLU	2.2
1	A	684	ILE	2.2
1	A	693	ILE	2.2
1	A	715	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	511	HIS	2.2
1	A	701	THR	2.2
1	A	3	GLU	2.2
1	A	870	ASP	2.2
1	A	741	ALA	2.1
1	A	638	PHE	2.1
1	A	882	LEU	2.1
1	A	658	ARG	2.1
1	A	792	ASP	2.1
1	A	892	GLY	2.1
1	A	284	GLY	2.0
1	A	745	PHE	2.0
1	A	515	VAL	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, 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
2	PO4	A	918	5/5	0.93	0.21	0.48	88,88,89,89	0
2	PO4	A	920	5/5	0.92	0.52	-	78,81,82,83	0
2	PO4	A	919	5/5	0.96	0.29	-	82,82,83,84	0

6.5 Other polymers (i)

There are no such residues in this entry.