Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:30 PM GMT

PDB ID	:	1TXK
Title	:	Crystal structure of Escherichia coli OpgG
Authors	:	Hanoulle, X.; Rollet, E.; Clantin, B.; Landrieu, I.; Odberg-Ferragut, C.; Lippens, G.; Bohin, J.P.; Villeret, V.
Deposited on	:	2004-07-05
Resolution	:	2.50 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:

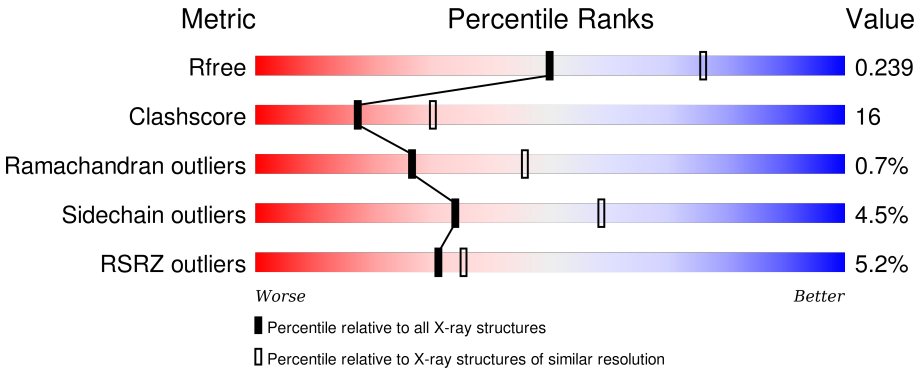
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	498	5% 71% 24%
1	B	498	5% 69% 25%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8291 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 Glucans biosynthesis protein G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	Se	0	0	0
			3922	2495	673	744	10			
1	B	487	Total	C	N	O	S	Se	0	0	0
			3891	2477	664	739	1	10			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	INITIATING METHIONINE	UNP P33136
A	54	MSE	MET	MODIFIED RESIDUE	UNP P33136
A	87	MSE	MET	MODIFIED RESIDUE	UNP P33136
A	151	MSE	MET	MODIFIED RESIDUE	UNP P33136
A	223	MSE	MET	MODIFIED RESIDUE	UNP P33136
A	253	MSE	MET	MODIFIED RESIDUE	UNP P33136
A	304	MSE	MET	MODIFIED RESIDUE	UNP P33136
A	379	MSE	MET	MODIFIED RESIDUE	UNP P33136
A	436	MSE	MET	MODIFIED RESIDUE	UNP P33136
A	475	MSE	MET	MODIFIED RESIDUE	UNP P33136
A	488	MSE	MET	MODIFIED RESIDUE	UNP P33136
A	512	VAL	-	EXPRESSION TAG	UNP P33136
A	513	GLU	-	EXPRESSION TAG	UNP P33136
A	514	HIS	-	EXPRESSION TAG	UNP P33136
A	515	HIS	-	EXPRESSION TAG	UNP P33136
A	516	HIS	-	EXPRESSION TAG	UNP P33136
A	517	HIS	-	EXPRESSION TAG	UNP P33136
A	518	HIS	-	EXPRESSION TAG	UNP P33136
A	519	HIS	-	EXPRESSION TAG	UNP P33136
B	22	MET	-	INITIATING METHIONINE	UNP P33136
B	54	MSE	MET	MODIFIED RESIDUE	UNP P33136
B	87	MSE	MET	MODIFIED RESIDUE	UNP P33136
B	151	MSE	MET	MODIFIED RESIDUE	UNP P33136
B	223	MSE	MET	MODIFIED RESIDUE	UNP P33136
B	253	MSE	MET	MODIFIED RESIDUE	UNP P33136

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Chain	Residue	Modelled	Actual	Comment	Reference
B	304	MSE	MET	MODIFIED RESIDUE	UNP P33136
B	379	MSE	MET	MODIFIED RESIDUE	UNP P33136
B	436	MSE	MET	MODIFIED RESIDUE	UNP P33136
B	475	MSE	MET	MODIFIED RESIDUE	UNP P33136
B	488	MSE	MET	MODIFIED RESIDUE	UNP P33136
B	512	VAL	-	EXPRESSION TAG	UNP P33136
B	513	GLU	-	EXPRESSION TAG	UNP P33136
B	514	HIS	-	EXPRESSION TAG	UNP P33136
B	515	HIS	-	EXPRESSION TAG	UNP P33136
B	516	HIS	-	EXPRESSION TAG	UNP P33136
B	517	HIS	-	EXPRESSION TAG	UNP P33136
B	518	HIS	-	EXPRESSION TAG	UNP P33136
B	519	HIS	-	EXPRESSION TAG	UNP P33136

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0

- Molecule 3 is water.

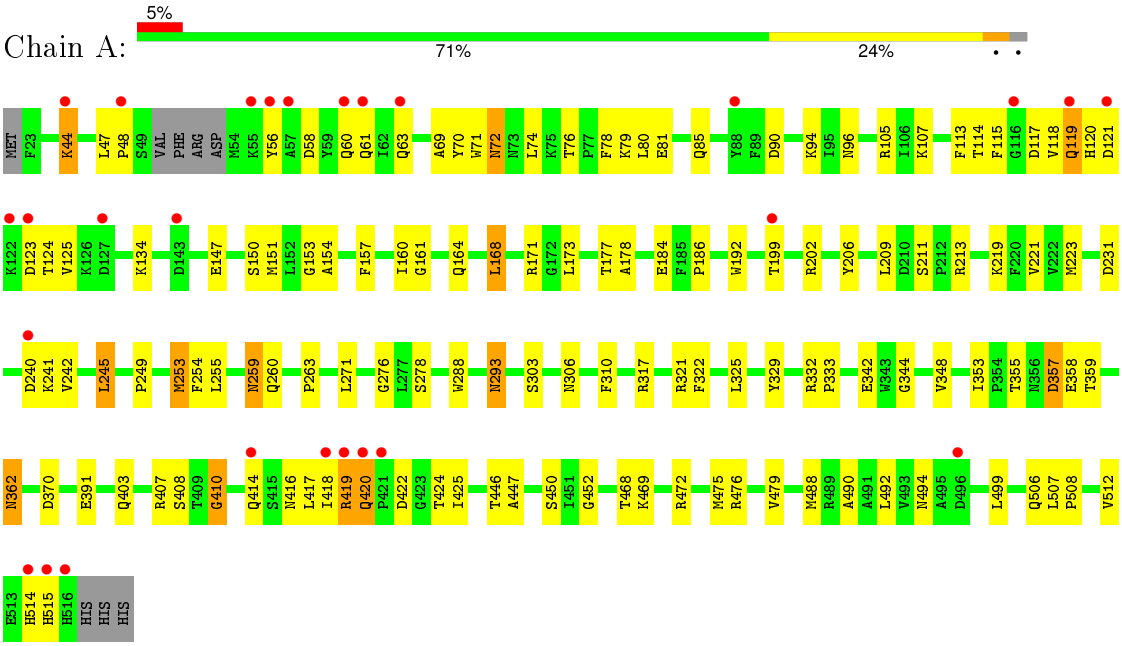
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	243	Total O 243 243	0	0
3	B	234	Total O 234 234	0	0

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.

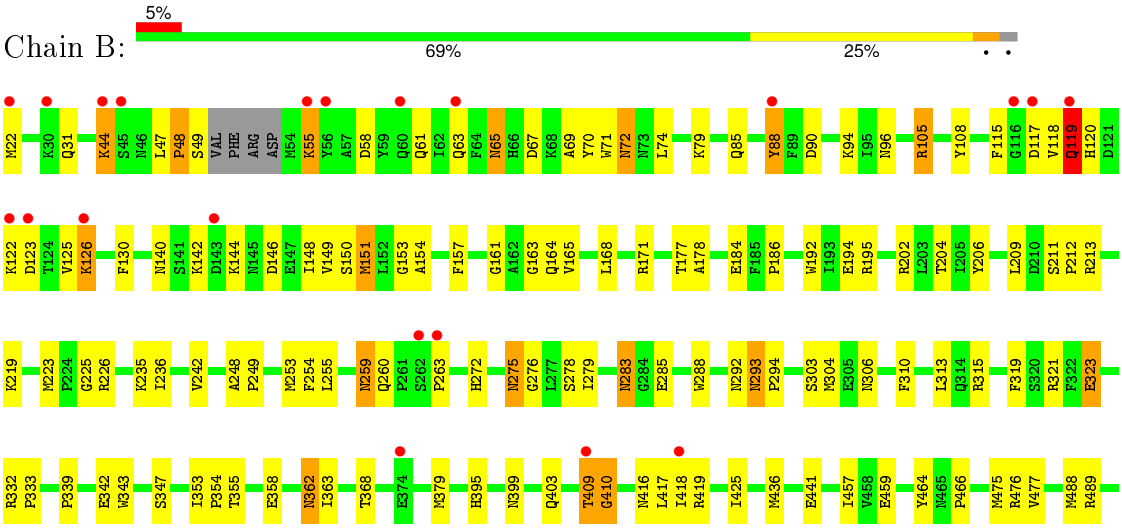
- Molecule 1: Glucans biosynthesis protein G

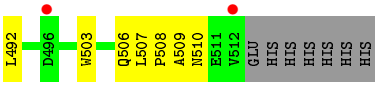
Chain A:



- Molecule 1: Glucans biosynthesis protein G

Chain B:




L492
D496
W503
Q506
L507
P508
A509
N510
E511
V512
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.86Å 88.12Å 215.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.99-2.50) 99.6 (20.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.18 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.192 , 0.229 0.206 , 0.239	Depositor DCC
R_{free} test set	4175 reflections (9.76%)	DCC
Wilson B-factor (Å^2)	36.3	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 80516 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8291	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.64% 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: NA

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	0.39	0/4017	0.67	4/5438 (0.1%)
1	B	0.37	0/3983	0.64	0/5391
All	All	0.38	0/8000	0.65	4/10829 (0.0%)

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	492	LEU	O-C-N	6.71	133.44	122.70
1	A	492	LEU	C-N-CA	-6.08	106.51	121.70
1	A	492	LEU	CA-C-N	-5.67	104.73	117.20
1	A	348	VAL	N-CA-C	-5.29	96.72	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	3922	0	3814	123	0
1	B	3891	0	3796	130	0
2	A	1	0	0	0	0
3	A	243	0	0	4	0
3	B	234	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8291	0	7610	248	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (248) 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:253:MSE:HE1	1:B:255:LEU:HB2	1.24	1.18
1:A:253:MSE:HE1	1:A:255:LEU:HB2	1.21	1.08
1:B:409:THR:HG23	1:B:410:GLY:H	1.11	1.06
1:B:253:MSE:HE3	1:B:358:GLU:HA	1.36	1.03
1:A:253:MSE:HE3	1:A:358:GLU:HA	1.36	1.02
1:B:140:ASN:HD21	1:B:163:GLY:H	1.11	0.94
1:B:253:MSE:CE	1:B:255:LEU:HB2	1.99	0.93
1:B:425:ILE:HD11	1:B:507:LEU:HD11	1.49	0.93
1:B:202:ARG:HG2	1:B:223:MSE:HG2	1.51	0.91
1:A:259:ASN:H	1:A:259:ASN:HD22	1.19	0.91
1:A:44:LYS:H	1:A:44:LYS:HE2	1.34	0.91
1:A:254:PHE:H	1:A:362:ASN:HD21	1.20	0.88
1:B:186:PRO:HB3	1:B:211:SER:HB2	1.58	0.86
1:B:409:THR:HG23	1:B:410:GLY:N	1.90	0.85
1:A:410:GLY:HA3	1:A:424:THR:HG23	1.59	0.84
1:B:259:ASN:HD22	1:B:259:ASN:H	1.23	0.83
1:B:409:THR:HG21	1:B:419:ARG:NH1	1.96	0.80
1:B:254:PHE:H	1:B:362:ASN:HD21	1.28	0.78
1:B:260:GLN:NE2	1:B:293:ASN:H	1.81	0.77
1:A:115:PHE:HB3	1:A:118:VAL:CG2	2.14	0.77
1:B:119:GLN:H	1:B:119:GLN:NE2	1.83	0.76
1:B:409:THR:HG21	1:B:419:ARG:CZ	2.15	0.76
1:A:422:ASP:OD1	1:A:424:THR:HG22	1.85	0.76
1:B:362:ASN:HD22	1:B:362:ASN:H	1.32	0.76
1:A:186:PRO:HB3	1:A:211:SER:HB2	1.67	0.75
1:A:362:ASN:H	1:A:362:ASN:HD22	1.33	0.75
1:A:306:ASN:ND2	1:A:344:GLY:H	1.84	0.75
1:B:409:THR:CG2	1:B:410:GLY:H	1.96	0.75
1:B:260:GLN:HE22	1:B:293:ASN:H	1.35	0.75
1:A:306:ASN:HD22	1:A:344:GLY:H	1.34	0.74
1:A:472:ARG:HH12	1:B:323:GLU:HG2	1.51	0.73
1:B:115:PHE:HB3	1:B:118:VAL:HB	1.70	0.73
1:A:253:MSE:HE1	1:A:255:LEU:CB	2.12	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ASN:HD22	1:A:105:ARG:HA	1.54	0.72
1:B:119:GLN:HG2	1:B:120:HIS:H	1.54	0.72
1:B:140:ASN:ND2	1:B:163:GLY:H	1.87	0.72
1:B:294:PRO:O	1:B:354:PRO:HB3	1.91	0.71
1:B:293:ASN:HD21	1:B:355:THR:H	1.40	0.70
1:B:192:TRP:HB2	1:B:206:TYR:HB2	1.74	0.70
1:A:446:THR:HG22	1:A:447:ALA:N	2.06	0.70
1:B:44:LYS:H	1:B:44:LYS:HD3	1.56	0.69
1:B:171:ARG:HB2	1:B:249:PRO:HG2	1.75	0.69
1:A:192:TRP:HB2	1:A:206:TYR:HB2	1.73	0.68
1:B:55:LYS:HE3	1:B:55:LYS:HA	1.76	0.68
1:A:317:ARG:NH2	1:A:332:ARG:O	2.23	0.68
1:A:410:GLY:CA	1:A:424:THR:HG23	2.23	0.68
1:B:279:ILE:HG21	1:B:304:MSE:HE1	1.77	0.67
1:B:123:ASP:O	1:B:126:LYS:HD2	1.94	0.66
1:A:44:LYS:H	1:A:44:LYS:CE	2.08	0.65
1:A:173:LEU:HD11	1:A:245:LEU:HD11	1.77	0.65
1:A:293:ASN:HD21	1:A:355:THR:H	1.44	0.65
1:B:403:GLN:HA	1:B:403:GLN:HE21	1.62	0.65
1:B:122:LYS:HE2	1:B:122:LYS:HA	1.77	0.65
1:B:202:ARG:HG3	1:B:202:ARG:HH21	1.62	0.64
1:A:403:GLN:HE21	1:A:403:GLN:HA	1.63	0.64
1:A:115:PHE:HB3	1:A:118:VAL:HG23	1.79	0.64
1:A:78:PHE:O	1:A:79:LYS:HD2	1.96	0.64
1:A:403:GLN:NE2	1:A:403:GLN:HA	2.12	0.64
1:B:475:MSE:HE1	1:B:488:MSE:HB2	1.79	0.64
1:B:184:GLU:OE1	1:B:213:ARG:HD3	1.98	0.64
1:B:403:GLN:NE2	1:B:403:GLN:HA	2.14	0.63
1:A:446:THR:HG22	1:A:447:ALA:H	1.64	0.63
1:B:319:PHE:CE1	1:B:323:GLU:HA	2.34	0.63
1:A:260:GLN:OE1	1:A:293:ASN:N	2.31	0.63
1:A:171:ARG:HB2	1:A:249:PRO:HG2	1.80	0.63
1:A:213:ARG:HH21	1:A:242:VAL:HA	1.64	0.63
1:A:47:LEU:HD21	1:A:85:GLN:HB3	1.80	0.62
1:A:475:MSE:HE1	1:A:490:ALA:HB2	1.81	0.62
1:B:425:ILE:CD1	1:B:507:LEU:HD11	2.27	0.62
1:A:362:ASN:HD22	1:A:362:ASN:N	1.99	0.61
1:A:259:ASN:ND2	1:A:259:ASN:H	1.96	0.60
1:B:362:ASN:N	1:B:362:ASN:HD22	1.99	0.60
1:B:253:MSE:HE3	1:B:358:GLU:CA	2.23	0.60
1:B:441:GLU:HG2	1:B:464:TYR:CE2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:ASN:HD21	1:B:315:ARG:H	1.48	0.60
1:B:276:GLY:HA3	1:B:288:TRP:CH2	2.36	0.60
1:B:236:ILE:HG13	1:B:379:MSE:HE3	1.83	0.59
1:A:422:ASP:CG	1:A:424:THR:HG22	2.23	0.59
1:B:441:GLU:HG2	1:B:464:TYR:CD2	2.38	0.59
1:A:263:PRO:HD2	1:B:417:LEU:HD22	1.84	0.59
1:A:115:PHE:HB3	1:A:118:VAL:HG22	1.82	0.59
1:A:417:LEU:HD22	1:B:263:PRO:HD2	1.85	0.58
1:A:107:LYS:HB2	1:A:107:LYS:NZ	2.20	0.57
1:A:260:GLN:HG3	1:A:260:GLN:O	2.04	0.56
1:B:259:ASN:ND2	1:B:259:ASN:H	1.99	0.56
1:B:260:GLN:HE21	1:B:292:ASN:HA	1.70	0.56
1:A:424:THR:HG21	1:A:476:ARG:HH21	1.71	0.56
1:A:119:GLN:O	1:A:120:HIS:ND1	2.39	0.56
1:B:259:ASN:HD22	1:B:259:ASN:N	2.01	0.55
1:B:353:ILE:O	1:B:362:ASN:HB2	2.07	0.55
1:B:459:GLU:HG2	1:B:476:ARG:HB3	1.88	0.55
1:A:276:GLY:HA3	1:A:288:TRP:CH2	2.42	0.54
1:A:253:MSE:HA	1:A:362:ASN:ND2	2.22	0.54
1:A:202:ARG:HG2	1:A:223:MSE:HG2	1.88	0.54
1:B:260:GLN:HG3	1:B:260:GLN:O	2.06	0.54
1:A:424:THR:HG21	1:A:476:ARG:HE	1.73	0.54
1:B:71:TRP:CD1	1:B:74:LEU:HD12	2.42	0.54
1:A:213:ARG:NH2	1:A:242:VAL:HA	2.23	0.54
1:B:65:ASN:C	1:B:65:ASN:HD22	2.09	0.54
1:A:121:ASP:HB2	1:A:124:THR:HG23	1.89	0.54
1:B:171:ARG:HB2	1:B:249:PRO:CG	2.37	0.53
1:B:283:ASN:ND2	1:B:285:GLU:H	2.04	0.53
1:A:424:THR:HG21	1:A:476:ARG:NH2	2.24	0.53
1:A:61:GLN:HG3	1:A:117:ASP:OD2	2.09	0.53
1:A:70:TYR:O	1:A:71:TRP:HB2	2.09	0.53
1:A:446:THR:CG2	1:A:447:ALA:N	2.72	0.53
1:B:416:ASN:OD1	1:B:418:ILE:HG12	2.08	0.52
1:B:260:GLN:NE2	1:B:292:ASN:HA	2.23	0.52
1:B:47:LEU:CD2	1:B:90:ASP:HA	2.38	0.52
1:A:58:ASP:O	1:A:61:GLN:HB2	2.10	0.51
1:B:303:SER:HA	1:B:347:SER:CB	2.40	0.51
1:B:275:ASN:H	1:B:275:ASN:HD22	1.58	0.51
1:A:186:PRO:HB3	1:A:211:SER:CB	2.37	0.51
1:B:164:GLN:OE1	1:B:333:PRO:HB3	2.11	0.51
1:A:472:ARG:NH1	1:B:323:GLU:HG2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LYS:N	1:B:44:LYS:HD3	2.25	0.51
1:B:368:THR:O	1:B:368:THR:HG23	2.10	0.51
1:A:44:LYS:HE2	1:A:44:LYS:N	2.16	0.50
1:A:410:GLY:HA3	1:A:424:THR:CG2	2.38	0.50
1:A:446:THR:CG2	1:A:447:ALA:H	2.24	0.50
1:A:47:LEU:CD1	1:A:90:ASP:HA	2.41	0.50
1:B:306:ASN:OD1	1:B:342:GLU:HB3	2.12	0.50
1:A:420:GLN:NE2	1:A:420:GLN:H	2.09	0.50
1:B:260:GLN:HE22	1:B:293:ASN:N	2.06	0.50
1:A:121:ASP:O	1:A:125:VAL:HG22	2.11	0.50
1:B:303:SER:HA	1:B:347:SER:HB3	1.94	0.50
1:B:395:HIS:HE1	1:B:399:ASN:OD1	1.95	0.50
1:B:177:THR:O	1:B:178:ALA:HB3	2.12	0.49
1:A:184:GLU:OE2	1:A:213:ARG:HD3	2.13	0.49
1:A:479:VAL:HG21	1:A:512:VAL:HG21	1.94	0.49
1:A:164:GLN:OE1	1:A:333:PRO:HB3	2.12	0.49
1:A:424:THR:HG21	1:A:476:ARG:NE	2.28	0.49
1:A:506:GLN:O	1:A:508:PRO:HD3	2.13	0.49
1:B:151:MSE:HE3	1:B:157:PHE:CG	2.48	0.49
1:B:319:PHE:CZ	1:B:323:GLU:HA	2.48	0.48
1:A:168:LEU:O	1:A:168:LEU:HD12	2.13	0.48
1:A:468:THR:O	1:A:469:LYS:HB2	2.13	0.48
1:A:71:TRP:CD1	1:A:74:LEU:HD12	2.49	0.48
1:B:119:GLN:H	1:B:119:GLN:HE21	1.59	0.48
1:B:63:GLN:HE21	1:B:63:GLN:HA	1.78	0.48
1:A:96:ASN:HD21	1:A:105:ARG:HD3	1.79	0.48
1:A:117:ASP:OD1	1:A:117:ASP:N	2.42	0.48
1:A:253:MSE:HE3	1:A:358:GLU:CA	2.26	0.48
1:A:403:GLN:CA	1:A:403:GLN:HE21	2.26	0.48
1:B:165:VAL:HG23	1:B:332:ARG:HG2	1.96	0.48
1:A:353:ILE:O	1:A:362:ASN:HB2	2.14	0.47
1:A:253:MSE:CE	1:A:255:LEU:HB2	2.15	0.47
1:B:47:LEU:HD21	1:B:85:GLN:NE2	2.29	0.47
1:B:58:ASP:HA	1:B:61:GLN:HE21	1.78	0.47
1:A:105:ARG:HG3	1:A:105:ARG:HH11	1.78	0.47
1:B:148:ILE:HG13	1:B:149:VAL:HG23	1.95	0.47
1:A:107:LYS:HB2	1:A:107:LYS:HZ2	1.80	0.47
1:A:276:GLY:HA3	1:A:288:TRP:CZ2	2.48	0.47
1:B:339:PRO:HB3	1:B:343:TRP:CE2	2.50	0.47
1:B:425:ILE:O	1:B:425:ILE:HG13	2.15	0.46
1:B:70:TYR:O	1:B:71:TRP:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:TYR:HA	1:B:130:PHE:CZ	2.50	0.46
1:A:96:ASN:ND2	1:A:105:ARG:HD3	2.31	0.46
1:B:194:GLU:CG	1:B:204:THR:HB	2.46	0.46
1:A:76:THR:O	1:A:79:LYS:NZ	2.44	0.46
1:A:47:LEU:HD11	1:A:90:ASP:HA	1.97	0.46
1:B:278:SER:HB2	1:B:313:LEU:HD22	1.98	0.46
1:A:357:ASP:OD2	1:A:359:THR:HG23	2.16	0.46
1:B:120:HIS:HA	1:B:125:VAL:CG1	2.46	0.46
1:A:69:ALA:HB3	1:A:72:ASN:CG	2.37	0.46
1:A:416:ASN:HD21	1:A:418:ILE:HG13	1.80	0.46
1:B:506:GLN:O	1:B:508:PRO:HD3	2.16	0.45
1:B:153:GLY:O	1:B:154:ALA:C	2.53	0.45
1:B:96:ASN:ND2	1:B:105:ARG:HD3	2.31	0.45
1:B:119:GLN:O	1:B:120:HIS:ND1	2.50	0.45
1:A:407:ARG:HG2	1:A:408:SER:N	2.31	0.45
1:B:117:ASP:OD1	1:B:117:ASP:O	2.34	0.45
1:B:409:THR:CG2	1:B:410:GLY:N	2.63	0.45
1:B:186:PRO:CB	1:B:211:SER:HB2	2.38	0.45
1:A:407:ARG:HG3	1:A:425:ILE:HD11	1.99	0.45
1:B:186:PRO:HB3	1:B:211:SER:CB	2.38	0.45
1:A:317:ARG:HD2	1:A:391:GLU:OE2	2.16	0.45
1:A:452:GLY:HA3	3:A:628:HOH:O	2.17	0.44
1:B:161:GLY:H	1:B:164:GLN:CD	2.20	0.44
1:A:221:VAL:HB	1:A:231:ASP:HB3	1.99	0.44
1:B:278:SER:O	1:B:310:PHE:HA	2.17	0.44
1:A:171:ARG:HB2	1:A:249:PRO:CG	2.45	0.44
1:B:219:LYS:HD3	3:B:622:HOH:O	2.17	0.44
1:B:69:ALA:HB3	1:B:72:ASN:ND2	2.33	0.44
1:B:436:MSE:HE1	1:B:492:LEU:HD23	1.99	0.44
1:A:47:LEU:HG	1:A:90:ASP:HA	2.00	0.44
1:B:61:GLN:NE2	1:B:117:ASP:OD1	2.49	0.44
1:A:419:ARG:HD3	1:A:420:GLN:N	2.33	0.44
1:B:362:ASN:ND2	1:B:363:ILE:HG12	2.33	0.44
1:A:424:THR:CG2	1:A:476:ARG:HE	2.31	0.43
1:B:213:ARG:NH2	1:B:242:VAL:HA	2.33	0.43
1:A:414:GLN:OE1	1:A:416:ASN:HB2	2.18	0.43
1:B:509:ALA:O	1:B:510:ASN:HB2	2.19	0.43
1:A:278:SER:O	1:A:310:PHE:HA	2.18	0.43
1:B:48:PRO:O	1:B:49:SER:C	2.57	0.43
1:A:121:ASP:C	1:A:123:ASP:H	2.20	0.43
1:A:494:ASN:HB2	1:A:499:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ARG:NH1	3:B:520:HOH:O	2.51	0.43
1:B:260:GLN:NE2	1:B:293:ASN:N	2.60	0.43
1:B:74:LEU:HD11	1:B:195:ARG:HD3	2.00	0.43
1:B:475:MSE:HE3	1:B:477:VAL:HG11	2.01	0.43
1:A:209:LEU:C	1:A:209:LEU:HD23	2.39	0.43
1:A:325:LEU:HD22	1:B:466:PRO:HD2	2.01	0.43
1:B:63:GLN:NE2	1:B:63:GLN:HA	2.33	0.43
1:B:65:ASN:C	1:B:65:ASN:ND2	2.73	0.43
1:B:209:LEU:HD23	1:B:209:LEU:C	2.40	0.42
1:A:81:GLU:HB2	1:A:134:LYS:CG	2.49	0.42
1:A:177:THR:O	1:A:178:ALA:HB3	2.18	0.42
1:B:276:GLY:HA3	1:B:288:TRP:CZ2	2.55	0.42
1:A:512:VAL:HG22	3:A:669:HOH:O	2.19	0.42
1:B:31:GLN:HA	1:B:31:GLN:NE2	2.34	0.42
1:A:322:PHE:CD2	1:A:329:TYR:HB2	2.53	0.42
1:A:115:PHE:CD2	1:A:120:HIS:HB3	2.54	0.42
1:A:306:ASN:ND2	1:A:342:GLU:HB3	2.34	0.42
1:A:514:HIS:ND1	1:A:515:HIS:N	2.68	0.42
1:A:206:TYR:CE1	1:A:219:LYS:HG3	2.54	0.42
1:B:144:LYS:HE3	1:B:146:ASP:OD1	2.20	0.42
1:B:65:ASN:ND2	1:B:67:ASP:H	2.18	0.42
1:B:457:ILE:HA	1:B:477:VAL:HG12	2.02	0.41
1:A:168:LEU:C	1:A:168:LEU:HD12	2.41	0.41
1:A:94:LYS:HE3	3:A:767:HOH:O	2.20	0.41
1:A:147:GLU:O	1:A:160:ILE:HD11	2.20	0.41
1:A:70:TYR:HB3	1:A:80:LEU:HB2	2.02	0.41
1:B:94:LYS:HZ2	1:B:105:ARG:HH21	1.69	0.41
1:B:94:LYS:NZ	1:B:105:ARG:HH21	2.18	0.41
1:A:113:PHE:CD1	1:A:113:PHE:N	2.88	0.41
1:B:150:SER:O	1:B:157:PHE:HA	2.20	0.41
1:B:235:LYS:HA	1:B:379:MSE:O	2.20	0.41
1:A:321:ARG:HD2	3:A:601:HOH:O	2.20	0.41
1:B:120:HIS:CG	1:B:120:HIS:O	2.74	0.41
1:A:115:PHE:CD1	1:A:115:PHE:N	2.89	0.41
1:B:142:LYS:HE2	1:B:142:LYS:HB3	1.69	0.41
1:A:150:SER:O	1:A:157:PHE:HA	2.21	0.41
1:B:225:GLY:O	1:B:226:ARG:C	2.59	0.41
1:B:416:ASN:HB3	1:B:419:ARG:HB2	2.03	0.41
1:A:119:GLN:HA	1:A:119:GLN:HE21	1.85	0.41
1:A:153:GLY:O	1:A:154:ALA:C	2.58	0.41
1:A:63:GLN:O	1:A:114:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:LEU:HD23	1:A:271:LEU:C	2.41	0.41
1:A:240:ASP:OD1	1:A:241:LYS:N	2.54	0.41
1:A:161:GLY:H	1:A:164:GLN:CD	2.24	0.40
1:B:508:PRO:HG3	3:B:559:HOH:O	2.20	0.40
1:B:88:TYR:CD1	1:B:88:TYR:N	2.85	0.40
1:A:56:TYR:C	1:A:56:TYR:CD1	2.93	0.40
1:A:422:ASP:OD2	1:A:424:THR:HG22	2.21	0.40
1:B:248:ALA:N	1:B:249:PRO:CD	2.84	0.40
1:B:489:ARG:HA	1:B:503:TRP:O	2.21	0.40
1:B:272:HIS:CE1	1:B:275:ASN:HB3	2.57	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	486/498 (98%)	464 (96%)	19 (4%)	3 (1%)	30	50
1	B	483/498 (97%)	457 (95%)	22 (5%)	4 (1%)	24	41
All	All	969/996 (97%)	921 (95%)	41 (4%)	7 (1%)	26	46

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	119	GLN
1	B	409	THR
1	A	48	PRO
1	A	119	GLN
1	A	410	GLY
1	B	48	PRO
1	B	410	GLY

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	425/423 (100%)	406 (96%)	19 (4%)	34 59
1	B	422/423 (100%)	403 (96%)	19 (4%)	34 59
All	All	847/846 (100%)	809 (96%)	38 (4%)	34 59

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LYS
1	A	60	GLN
1	A	72	ASN
1	A	151	MSE
1	A	168	LEU
1	A	199	THR
1	A	245	LEU
1	A	253	MSE
1	A	259	ASN
1	A	293	ASN
1	A	303	SER
1	A	357	ASP
1	A	362	ASN
1	A	370	ASP
1	A	419	ARG
1	A	420	GLN
1	A	450	SER
1	A	488	MSE
1	A	507	LEU
1	B	22	MET
1	B	44	LYS
1	B	55	LYS
1	B	65	ASN
1	B	72	ASN
1	B	79	LYS
1	B	88	TYR
1	B	105	ARG

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Mol	Chain	Res	Type
1	B	119	GLN
1	B	126	LYS
1	B	151	MSE
1	B	168	LEU
1	B	212	PRO
1	B	259	ASN
1	B	275	ASN
1	B	283	ASN
1	B	293	ASN
1	B	323	GLU
1	B	362	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	72	ASN
1	A	96	ASN
1	A	119	GLN
1	A	145	ASN
1	A	259	ASN
1	A	292	ASN
1	A	293	ASN
1	A	306	ASN
1	A	362	ASN
1	A	403	GLN
1	A	416	ASN
1	A	420	GLN
1	A	506	GLN
1	A	510	ASN
1	B	31	GLN
1	B	63	GLN
1	B	65	ASN
1	B	72	ASN
1	B	96	ASN
1	B	119	GLN
1	B	140	ASN
1	B	233	GLN
1	B	259	ASN
1	B	260	GLN
1	B	275	ASN
1	B	283	ASN

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Mol	Chain	Res	Type
1	B	293	ASN
1	B	362	ASN
1	B	371	GLN
1	B	395	HIS
1	B	403	GLN
1	B	414	GLN
1	B	497	GLN
1	B	506	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

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

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	480/498 (96%)	0.18	27 (5%)	28	31	19, 32, 63, 82	0
1	B	477/498 (95%)	0.15	23 (4%)	34	39	20, 33, 57, 78	0
All	All	957/996 (96%)	0.17	50 (5%)	31	35	19, 33, 60, 82	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	515	HIS	9.0
1	B	119	GLN	7.2
1	A	514	HIS	7.1
1	A	420	GLN	6.3
1	B	123	ASP	6.0
1	A	123	ASP	5.4
1	A	55	LYS	5.3
1	A	122	LYS	5.3
1	B	117	ASP	5.1
1	A	119	GLN	4.5
1	A	44	LYS	4.0
1	A	421	PRO	3.9
1	A	418	ILE	3.9
1	B	55	LYS	3.8
1	B	88	TYR	3.7
1	B	122	LYS	3.7
1	B	44	LYS	3.6
1	A	496	ASP	3.6
1	A	121	ASP	3.5
1	B	263	PRO	3.5
1	A	419	ARG	3.5
1	A	116	GLY	3.4
1	A	61	GLN	3.3
1	B	56	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	143	ASP	3.2
1	B	512	VAL	3.1
1	B	60	GLN	3.0
1	B	22	MET	2.9
1	A	127	ASP	2.9
1	B	116	GLY	2.6
1	A	88	TYR	2.6
1	B	30	LYS	2.5
1	B	126	LYS	2.5
1	B	409	THR	2.4
1	A	48	PRO	2.4
1	B	418	ILE	2.4
1	B	143	ASP	2.4
1	A	516	HIS	2.4
1	B	262	SER	2.3
1	B	374	GLU	2.3
1	A	414	GLN	2.3
1	B	45	SER	2.3
1	A	199	THR	2.3
1	B	63	GLN	2.3
1	A	60	GLN	2.2
1	B	496	ASP	2.2
1	A	57	ALA	2.2
1	A	63	GLN	2.1
1	A	56	TYR	2.1
1	A	240	ASP	2.1

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	NA	A	600	1/1	0.88	0.19	-	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.