Full wwPDB X-ray Structure Validation Report (i)

Jan 19, 2017 – 01:12 PM EST

PDB ID	:	4C0S
Title	:	Mammalian translation elongation factor eEF1A2
Authors	:	Crepin, T.; Shalak, V.F.; Yaremchuk, A.D.; Vlasenko, D.O.; McCarthy, A.A.; Negrutskii, B.S.; Tukalo, M.A.; El'skaya, A.V.
Deposited on	:	2013-08-07
Resolution	:	2.70 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:

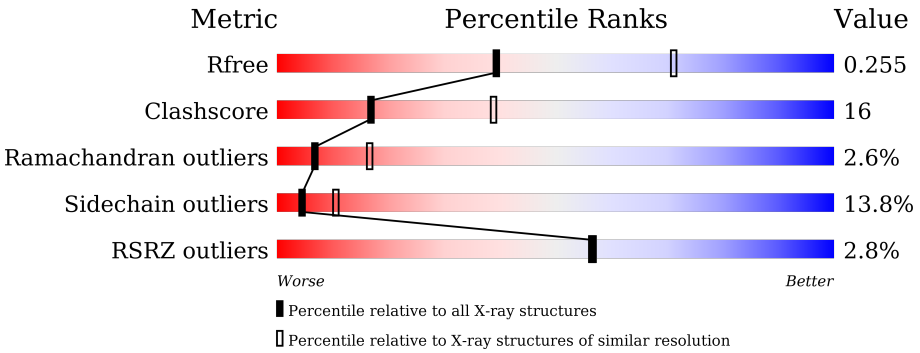
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	463	4% 60% 30% 6% ·
1	B	463	% 62% 27% 6% 5%

2 Entry composition

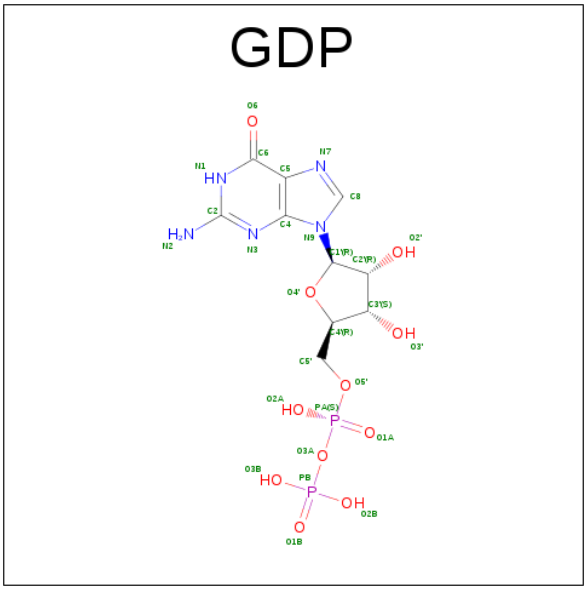
There are 4 unique types of molecules in this entry. The entry contains 6951 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ELONGATION FACTOR 1-ALPHA 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	P	S	0	0	0
			3470	2196	600	656	2	16			
1	B	442	Total	C	N	O	P	S	0	0	0
			3414	2162	589	645	2	16			

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is water.

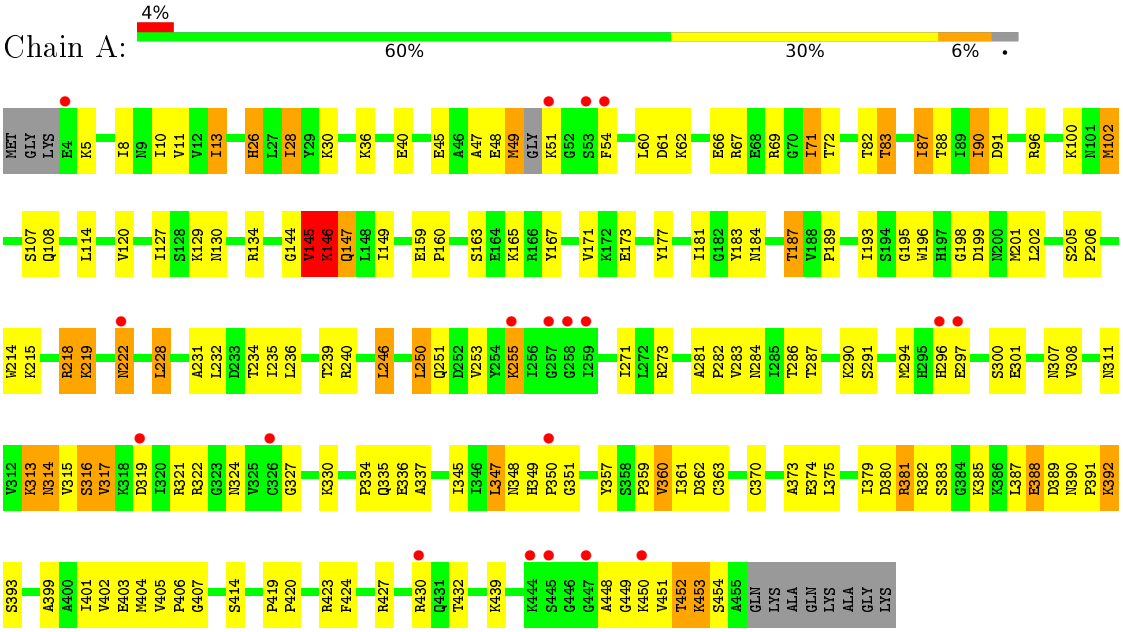
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total O 3 3	0	0
4	B	6	Total O 6 6	0	0

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.

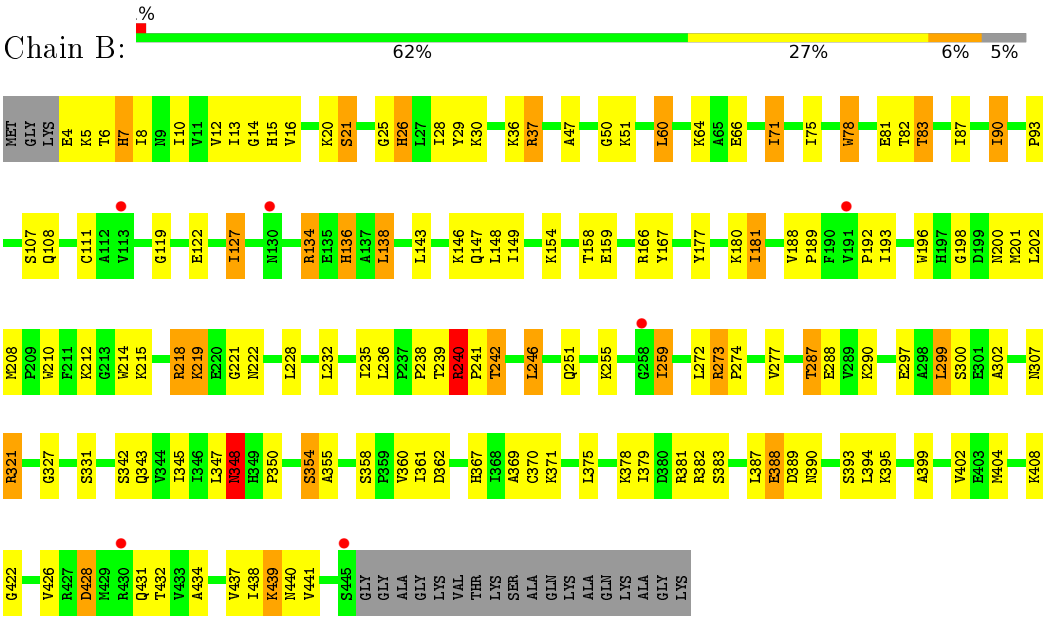
- Molecule 1: ELONGATION FACTOR 1-ALPHA 2

Chain A:



- Molecule 1: ELONGATION FACTOR 1-ALPHA 2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	135.37Å 135.37Å 304.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.70 24.81 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (25.00-2.70) 99.0 (24.81-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.6.0114	Depositor
R, R_{free}	0.202 , 0.256 0.203 , 0.255	Depositor DCC
R_{free} test set	2299 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	58.8	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6951	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: GDP, TPO, MG, SEP

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	0.73	1/3517 (0.0%)	0.65	0/4751
1	B	0.84	3/3462 (0.1%)	0.73	1/4680 (0.0%)
All	All	0.79	4/6979 (0.1%)	0.69	1/9431 (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	1
1	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	214	TRP	CD2-CE2	7.00	1.49	1.41
1	B	196	TRP	CD2-CE2	6.23	1.48	1.41
1	A	196	TRP	CD2-CE2	5.08	1.47	1.41
1	B	78	TRP	CD2-CE2	5.02	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	240	ARG	NE-CZ-NH1	5.57	123.08	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	VAL	Peptide
1	B	238	PRO	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	3470	0	3521	120	0
1	B	3414	0	3457	117	0
2	A	28	0	12	0	0
2	B	28	0	12	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	3	0	0	0	0
4	B	6	0	0	0	0
All	All	6951	0	7002	229	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 (229) 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:145:VAL:HA	1:A:146:LYS:HB2	1.32	1.11
1:B:240:ARG:HG3	1:B:240:ARG:HH11	1.23	1.02
1:B:147:GLN:NE2	1:B:236:LEU:H	1.58	1.00
1:B:102:MET:HE2	1:B:107:SER:HB2	1.49	0.94
1:A:281:ALA:HB2	1:A:334:PRO:O	1.69	0.92
1:A:5:LYS:HE2	1:A:83:THR:O	1.69	0.90
1:B:147:GLN:HE22	1:B:236:LEU:H	1.18	0.88
1:A:30:LYS:HB3	1:A:202:LEU:HD11	1.57	0.86
1:A:145:VAL:CA	1:A:146:LYS:HB2	2.06	0.85
1:B:147:GLN:NE2	1:B:236:LEU:N	2.25	0.84
1:A:313:LYS:O	1:A:314:ASN:HB2	1.76	0.83
1:A:357:TYR:CE2	1:A:359:PRO:HG3	2.13	0.82
1:A:102:MET:HA	1:A:102:MET:HE3	1.58	0.82
1:B:14:GLY:H	1:B:136:HIS:HD2	1.27	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:VAL:HA	1:A:146:LYS:CB	2.09	0.81
1:B:127:ILE:HG13	1:B:134:ARG:HD2	1.63	0.81
1:A:449:GLY:HA2	1:A:450:LYS:C	2.01	0.80
1:B:251:GLN:HE22	1:B:307:ASN:HD21	1.28	0.80
1:A:177:TYR:CZ	1:A:181:ILE:HD11	2.19	0.78
1:A:251:GLN:HE22	1:A:307:ASN:HD21	1.31	0.78
1:B:5:LYS:NZ	1:B:81:GLU:OE2	2.17	0.76
1:A:375:LEU:O	1:A:391:PRO:HD2	1.87	0.75
1:B:387:LEU:O	1:B:388:GLU:HB2	1.86	0.74
1:A:167:TYR:O	1:A:171:VAL:HG23	1.86	0.74
1:A:452:THR:O	1:A:454:SER:N	2.20	0.73
1:B:102:MET:CE	1:B:107:SER:HB2	2.18	0.73
1:A:45:GLU:OE2	1:B:367:HIS:HE1	1.72	0.73
1:B:219:LYS:CD	1:B:219:LYS:H	2.02	0.72
1:B:10:ILE:HD13	1:B:111:CYS:HB3	1.71	0.72
1:A:321:ARG:NH2	1:B:37:ARG:HH22	1.88	0.71
1:A:177:TYR:OH	1:A:181:ILE:HD11	1.91	0.71
1:B:14:GLY:H	1:B:136:HIS:CD2	2.08	0.71
1:B:5:LYS:HE2	1:B:83:THR:O	1.91	0.71
1:A:294:MET:HB2	1:A:308:VAL:HG12	1.72	0.70
1:A:357:TYR:HE2	1:A:359:PRO:HG3	1.53	0.70
1:A:218:ARG:NH1	1:A:236:LEU:HD21	2.07	0.70
1:B:10:ILE:CD1	1:B:111:CYS:HB3	2.21	0.70
1:B:414:SER:HB2	1:B:439:LYS:O	1.91	0.70
1:A:419:PRO:HB2	1:A:420:PRO:HD3	1.74	0.69
1:A:222:ASN:HD22	1:A:222:ASN:N	1.92	0.67
1:A:282:PRO:HD2	1:A:324:ASN:HD22	1.59	0.67
1:B:154:LYS:HG2	2:B:500:GDP:C6	2.30	0.67
1:A:219:LYS:HE2	1:A:219:LYS:H	1.60	0.66
1:B:240:ARG:HG3	1:B:240:ARG:NH1	1.98	0.66
1:B:246:LEU:HD13	1:B:327:GLY:HA2	1.79	0.65
1:B:93:PRO:HG3	1:B:136:HIS:NE2	2.11	0.65
1:B:96:ARG:HG2	1:B:381:ARG:NH1	2.12	0.65
1:A:250:LEU:HD22	1:A:324:ASN:HB2	1.78	0.65
1:B:202:LEU:HD23	1:B:202:LEU:N	2.12	0.65
1:A:184:ASN:HB3	1:A:187:THR:HG23	1.79	0.64
1:B:47:ALA:O	1:B:50:GLY:O	2.16	0.64
1:A:360:VAL:HG23	1:A:427:ARG:O	1.97	0.64
1:B:127:ILE:HG13	1:B:134:ARG:CD	2.28	0.64
1:B:219:LYS:H	1:B:219:LYS:CE	2.10	0.64
1:A:5:LYS:CE	1:A:83:THR:O	2.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ILE:HD11	1:B:432:THR:HG21	1.81	0.63
1:B:240:ARG:CG	1:B:240:ARG:HH11	2.06	0.63
1:A:67:ARG:NH2	1:A:90:ILE:HD13	2.13	0.63
1:A:102:MET:HA	1:A:102:MET:CE	2.29	0.63
1:B:30:LYS:HB3	1:B:202:LEU:HD11	1.79	0.63
1:A:177:TYR:CE2	1:A:181:ILE:HD11	2.35	0.62
1:A:282:PRO:HD2	1:A:324:ASN:ND2	2.14	0.61
1:A:102:MET:HE3	1:A:107:SER:O	2.00	0.61
1:A:349:HIS:CD2	1:A:350:PRO:HD2	2.36	0.61
1:B:219:LYS:HE2	1:B:219:LYS:H	1.66	0.61
1:B:362:ASP:OD1	1:B:367:HIS:CD2	2.54	0.60
1:B:13:ILE:HD12	1:B:136:HIS:HB3	1.82	0.60
1:A:388:GLU:OE2	1:A:391:PRO:HA	2.02	0.60
1:B:287:THR:HG23	1:B:288:GLU:N	2.16	0.60
1:B:321:ARG:HG2	1:B:321:ARG:HH11	1.66	0.60
1:B:402:VAL:HG21	1:B:404:MET:HE2	1.82	0.60
1:A:251:GLN:HE22	1:A:307:ASN:ND2	2.00	0.59
1:B:222:ASN:HD22	1:B:222:ASN:N	2.01	0.59
1:A:11:VAL:HG23	1:A:91:ASP:O	2.02	0.59
1:A:13:ILE:HG13	1:A:114:LEU:HD13	1.83	0.59
1:B:15:HIS:HD2	1:B:16:VAL:O	1.85	0.58
1:B:147:GLN:HE21	1:B:235:ILE:HG23	1.68	0.58
1:B:428:ASP:O	1:B:431:GLN:HB2	2.03	0.58
1:A:222:ASN:HD22	1:A:222:ASN:H	1.52	0.57
1:A:282:PRO:HB3	1:A:336:GLU:HG3	1.86	0.57
1:B:354:SER:O	1:B:355:ALA:C	2.41	0.57
1:A:282:PRO:CB	1:A:336:GLU:HG3	2.35	0.57
1:A:383:SER:OG	1:A:385:LYS:HB2	2.03	0.57
1:B:201:MET:C	1:B:202:LEU:HD23	2.24	0.57
1:B:203:GLU:HB2	1:B:204:PRO:CD	2.35	0.57
1:A:336:GLU:HG2	1:A:337:ALA:N	2.20	0.56
1:A:96:ARG:CZ	1:A:381:ARG:HH22	2.18	0.56
1:B:360:VAL:HA	1:B:369:ALA:HA	1.88	0.56
1:B:273:ARG:HB2	1:B:274:PRO:CD	2.36	0.55
1:A:414:SER:HB2	1:A:439:LYS:O	2.07	0.55
1:A:250:LEU:CD2	1:A:324:ASN:HB2	2.36	0.55
1:A:321:ARG:HH21	1:B:37:ARG:HH22	1.53	0.55
1:A:184:ASN:HB3	1:A:187:THR:CG2	2.36	0.54
1:A:127:ILE:O	1:A:134:ARG:HD2	2.08	0.54
1:B:273:ARG:HB2	1:B:274:PRO:HD2	1.88	0.54
1:B:375:LEU:HD13	1:B:394:LEU:HG	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:LYS:HB3	1:A:452:THR:HG23	1.90	0.54
1:A:362:ASP:OD2	1:A:427:ARG:HD2	2.06	0.54
1:A:361:ILE:HG12	1:A:370:CYS:HB2	1.90	0.53
1:A:26:HIS:HD2	1:A:195:GLY:O	1.91	0.53
1:A:246:LEU:HG	1:A:271:ILE:O	2.07	0.53
1:A:321:ARG:N	1:A:324:ASN:OD1	2.42	0.53
1:B:219:LYS:H	1:B:219:LYS:HD2	1.73	0.53
1:A:291:SER:HB3	1:A:311:ASN:HB3	1.90	0.53
1:B:408:LYS:HB3	1:B:409:PRO:HD2	1.91	0.53
1:B:138:LEU:HD22	1:B:181:ILE:HD11	1.90	0.53
1:B:119:GLY:HA3	1:B:122:GLU:OE1	2.08	0.52
1:A:134:ARG:HB3	1:A:177:TYR:CZ	2.44	0.52
1:A:380:ASP:OD1	1:A:382:ARG:N	2.36	0.52
1:B:388:GLU:HG2	1:B:389:ASP:O	2.09	0.52
1:A:62:LYS:O	1:A:66:GLU:HG3	2.09	0.52
1:B:136:HIS:HE1	1:B:383:SER:O	1.92	0.52
1:A:273:ARG:HH21	1:A:301:GLU:HG2	1.74	0.52
1:A:239:TPO:O	1:A:239:TPO:HG23	2.10	0.52
1:A:375:LEU:O	1:A:390:ASN:HA	2.09	0.52
1:B:102:MET:HB3	1:B:143:LEU:HD11	1.92	0.51
1:A:26:HIS:HB3	1:A:201:MET:HE1	1.92	0.51
1:A:48:GLU:OE1	1:A:48:GLU:N	2.43	0.51
1:A:10:ILE:HG12	1:A:87:ILE:CG2	2.41	0.51
1:A:286:THR:HG22	1:A:287:THR:N	2.26	0.51
1:A:145:VAL:CA	1:A:146:LYS:CB	2.77	0.50
1:A:100:LYS:HB2	1:A:345:ILE:HD13	1.93	0.50
1:B:402:VAL:HG21	1:B:404:MET:CE	2.42	0.50
1:B:362:ASP:OD1	1:B:367:HIS:HD2	1.94	0.50
1:B:361:ILE:HD12	1:B:426:VAL:HG22	1.93	0.50
1:B:203:GLU:HB2	1:B:204:PRO:HD2	1.94	0.50
1:B:347:LEU:O	1:B:348:ASN:C	2.50	0.50
1:B:387:LEU:O	1:B:388:GLU:CB	2.57	0.49
1:B:158:THR:HG22	1:B:166:ARG:HG2	1.92	0.49
1:B:71:ILE:H	1:B:71:ILE:HD12	1.76	0.49
1:B:222:ASN:N	1:B:222:ASN:ND2	2.59	0.49
1:A:96:ARG:NH2	1:A:381:ARG:HH22	2.11	0.49
1:A:379:ILE:HB	1:A:399:ALA:HB3	1.95	0.49
1:B:138:LEU:HD12	1:B:138:LEU:O	2.12	0.48
1:A:47:ALA:C	1:A:48:GLU:OE1	2.51	0.48
1:A:149:ILE:HG12	1:A:189:PRO:HG2	1.95	0.48
1:A:234:THR:O	1:A:235:ILE:C	2.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:SER:HA	1:B:370:CYS:O	2.12	0.48
1:B:90:ILE:HG23	1:B:107:SER:HB3	1.95	0.48
1:A:214:TRP:CH2	1:A:234:THR:HG21	2.49	0.48
1:A:336:GLU:HG2	1:A:337:ALA:H	1.78	0.48
1:A:82:THR:O	1:A:83:THR:C	2.50	0.48
1:A:96:ARG:CZ	1:A:381:ARG:NH2	2.77	0.47
1:A:147:GLN:OE1	1:A:236:LEU:HG	2.14	0.47
1:B:148:LEU:O	1:B:188:VAL:HG13	2.13	0.47
1:A:255:LYS:HE2	1:A:317:VAL:CG1	2.45	0.47
1:B:20:LYS:HB2	1:B:20:LYS:HE2	1.65	0.46
1:B:154:LYS:HG2	2:B:500:GDP:C5	2.50	0.46
1:A:296:HIS:O	1:A:297:GLU:HG3	2.14	0.46
1:B:149:ILE:HG12	1:B:189:PRO:HG2	1.97	0.46
1:A:146:LYS:HD3	1:A:147:GLN:N	2.30	0.46
1:B:102:MET:CE	1:B:107:SER:CB	2.90	0.46
1:A:427:ARG:CZ	1:B:66:GLU:HG2	2.45	0.46
1:A:363:CYS:HB2	1:A:424:PHE:HB3	1.97	0.46
1:A:45:GLU:OE2	1:B:367:HIS:CE1	2.61	0.46
1:B:90:ILE:HA	1:B:90:ILE:HD12	1.72	0.46
1:B:361:ILE:CD1	1:B:426:VAL:HG22	2.46	0.45
1:A:28:ILE:HD13	1:A:28:ILE:HA	1.61	0.45
1:B:273:ARG:CB	1:B:300:SER:O	2.65	0.45
1:B:13:ILE:HB	1:B:136:HIS:CD2	2.52	0.45
1:B:255:LYS:HB2	1:B:317:VAL:HG21	1.99	0.45
1:A:432:THR:HG21	1:B:71:ILE:HD11	1.99	0.45
1:A:60:LEU:O	1:A:61:ASP:C	2.55	0.45
1:B:82:THR:HG23	1:B:87:ILE:HD12	1.99	0.45
1:B:93:PRO:HG3	1:B:136:HIS:CD2	2.51	0.45
1:B:426:VAL:HB	1:B:434:ALA:HB3	1.98	0.45
1:A:449:GLY:HA2	1:A:451:VAL:N	2.31	0.45
1:A:102:MET:CE	1:A:107:SER:O	2.65	0.44
1:A:380:ASP:C	1:A:380:ASP:OD1	2.55	0.44
1:A:451:VAL:HG12	1:A:451:VAL:O	2.18	0.44
1:B:158:THR:CG2	1:B:166:ARG:HG2	2.47	0.44
1:A:214:TRP:HH2	1:A:234:THR:CG2	2.31	0.44
1:B:82:THR:CG2	1:B:87:ILE:HD12	2.47	0.44
1:B:342:SER:HB2	1:B:437:VAL:O	2.18	0.44
1:A:347:LEU:O	1:A:349:HIS:N	2.51	0.44
1:B:147:GLN:NE2	1:B:235:ILE:HA	2.33	0.44
1:B:154:LYS:HE2	2:B:500:GDP:C4	2.53	0.44
1:B:273:ARG:HB2	1:B:300:SER:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:GLN:O	1:A:322:ARG:HB2	2.18	0.43
1:B:12:VAL:O	1:B:93:PRO:HD2	2.18	0.43
1:B:218:ARG:NH1	1:B:221:GLY:O	2.52	0.43
1:A:198:GLY:O	1:A:199:ASP:C	2.57	0.43
1:A:315:VAL:HG13	1:A:319:ASP:HB2	2.00	0.43
1:A:26:HIS:HB3	1:A:201:MET:CE	2.49	0.43
1:B:134:ARG:HH11	1:B:134:ARG:HG2	1.83	0.43
1:B:240:ARG:HA	1:B:241:PRO:HD2	1.93	0.43
1:B:60:LEU:O	1:B:64:LYS:HG3	2.19	0.43
1:B:321:ARG:NH1	1:B:321:ARG:HG2	2.34	0.42
1:A:144:GLY:O	1:A:146:LYS:HB2	2.19	0.42
1:B:402:VAL:CG2	1:B:404:MET:CE	2.97	0.42
1:A:316:SER:O	1:A:317:VAL:C	2.58	0.42
1:A:239:TPO:O	1:A:239:TPO:CG2	2.67	0.42
1:B:192:PRO:C	1:B:193:ILE:HG23	2.39	0.42
1:A:205:SER:HA	1:A:206:PRO:HD2	1.82	0.42
1:A:349:HIS:CE1	1:A:351:GLY:H	2.38	0.42
1:A:69:ARG:HA	1:A:69:ARG:HD2	1.85	0.42
1:B:208:MET:HG2	1:B:210:TRP:CZ2	2.55	0.42
1:B:26:HIS:HB3	1:B:201:MET:HE1	2.02	0.42
1:A:159:GLU:HA	1:A:160:PRO:HA	1.80	0.42
1:A:419:PRO:CB	1:A:420:PRO:HD3	2.47	0.42
1:A:405:VAL:HA	1:A:406:PRO:HD3	1.89	0.42
1:B:26:HIS:O	1:B:29:TYR:HB2	2.21	0.41
1:B:272:LEU:HB3	1:B:302:ALA:HB3	2.02	0.41
1:A:374:GLU:HB2	1:A:403:GLU:HG3	2.03	0.41
1:B:146:LYS:HE2	1:B:239:TPO:O3P	2.20	0.41
1:B:177:TYR:CZ	1:B:181:ILE:HG12	2.55	0.41
1:B:200:ASN:HA	1:B:203:GLU:O	2.20	0.41
1:B:75:ILE:HA	1:B:78:TRP:CE3	2.55	0.41
1:A:387:LEU:HA	1:A:387:LEU:HD23	1.83	0.41
1:A:451:VAL:O	1:A:452:THR:C	2.59	0.41
1:A:49:MET:HG3	1:A:49:MET:H	1.67	0.41
1:B:218:ARG:CG	1:B:218:ARG:HH11	2.34	0.41
1:B:7:HIS:O	1:B:8:ILE:HD13	2.20	0.41
1:B:198:GLY:O	1:B:201:MET:HG3	2.20	0.41
1:B:402:VAL:HG23	1:B:404:MET:HG3	2.03	0.41
1:A:321:ARG:CZ	1:B:37:ARG:HH22	2.33	0.41
1:B:422:GLY:O	1:B:438:ILE:HG13	2.20	0.41
1:A:145:VAL:O	1:A:183:TYR:OH	2.27	0.41
1:B:379:ILE:HB	1:B:399:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:SEP:O1P	1:A:165:LYS:HE2	2.21	0.41
1:A:402:VAL:HG21	1:A:404:MET:HE2	2.03	0.41
1:B:167:TYR:CD1	1:B:192:PRO:HB3	2.55	0.40
1:B:297:GLU:O	1:B:299:LEU:HD23	2.22	0.40
1:A:392:LYS:HG2	1:A:393:SER:H	1.86	0.40
1:B:25:GLY:O	1:B:29:TYR:CD1	2.75	0.40
1:A:228:LEU:O	1:A:231:ALA:HB3	2.21	0.40
1:A:246:LEU:HD13	1:A:327:GLY:HA2	2.03	0.40
1:B:21:SER:HA	1:B:60:LEU:HB2	2.04	0.40
1:A:255:LYS:HE2	1:A:317:VAL:HG12	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	445/463 (96%)	384 (86%)	48 (11%)	13 (3%)	6	14
1	B	438/463 (95%)	397 (91%)	31 (7%)	10 (2%)	8	20
All	All	883/926 (95%)	781 (88%)	79 (9%)	23 (3%)	7	16

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	VAL
1	A	348	ASN
1	A	448	ALA
1	A	452	THR
1	A	453	LYS
1	B	240	ARG
1	B	331	SER
1	B	350	PRO

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Mol	Chain	Res	Type
1	A	146	LYS
1	A	373	ALA
1	B	242	THR
1	B	388	GLU
1	B	348	ASN
1	A	240	ARG
1	A	284	ASN
1	A	314	ASN
1	B	439	LYS
1	B	390	ASN
1	A	407	GLY
1	B	259	ILE
1	A	145	VAL
1	B	317	VAL
1	A	283	VAL

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	376/383 (98%)	325 (86%)	51 (14%)	5 11
1	B	371/383 (97%)	319 (86%)	52 (14%)	4 10
All	All	747/766 (98%)	644 (86%)	103 (14%)	4 10

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	13	ILE
1	A	26	HIS
1	A	28	ILE
1	A	36	LYS
1	A	40	GLU
1	A	49	MET
1	A	51	LYS

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Mol	Chain	Res	Type
1	A	54	PHE
1	A	71	ILE
1	A	72	THR
1	A	83	THR
1	A	87	ILE
1	A	88	THR
1	A	90	ILE
1	A	102	MET
1	A	108	GLN
1	A	120	VAL
1	A	129	LYS
1	A	130	ASN
1	A	146	LYS
1	A	147	GLN
1	A	173	GLU
1	A	187	THR
1	A	193	ILE
1	A	215	LYS
1	A	218	ARG
1	A	219	LYS
1	A	222	ASN
1	A	228	LEU
1	A	232	LEU
1	A	246	LEU
1	A	250	LEU
1	A	253	VAL
1	A	255	LYS
1	A	290	LYS
1	A	300	SER
1	A	313	LYS
1	A	316	SER
1	A	330	LYS
1	A	335	GLN
1	A	347	LEU
1	A	360	VAL
1	A	381	ARG
1	A	388	GLU
1	A	389	ASP
1	A	392	LYS
1	A	401	ILE
1	A	423	ARG
1	A	430	ARG

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Mol	Chain	Res	Type
1	A	453	LYS
1	B	4	GLU
1	B	6	THR
1	B	7	HIS
1	B	21	SER
1	B	26	HIS
1	B	28	ILE
1	B	36	LYS
1	B	37	ARG
1	B	51	LYS
1	B	60	LEU
1	B	71	ILE
1	B	83	THR
1	B	90	ILE
1	B	108	GLN
1	B	127	ILE
1	B	134	ARG
1	B	136	HIS
1	B	138	LEU
1	B	159	GLU
1	B	180	LYS
1	B	181	ILE
1	B	203	GLU
1	B	205	SER
1	B	212	LYS
1	B	215	LYS
1	B	218	ARG
1	B	219	LYS
1	B	228	LEU
1	B	232	LEU
1	B	240	ARG
1	B	242	THR
1	B	246	LEU
1	B	259	ILE
1	B	273	ARG
1	B	277	VAL
1	B	287	THR
1	B	290	LYS
1	B	299	LEU
1	B	316	SER
1	B	321	ARG
1	B	343	GLN

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Mol	Chain	Res	Type
1	B	345	ILE
1	B	348	ASN
1	B	354	SER
1	B	371	LYS
1	B	378	LYS
1	B	382	ARG
1	B	393	SER
1	B	395	LYS
1	B	428	ASP
1	B	440	ASN
1	B	441	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	132	GLN
1	A	222	ASN
1	A	295	HIS
1	A	307	ASN
1	A	349	HIS
1	B	26	HIS
1	B	132	GLN
1	B	136	HIS
1	B	147	GLN
1	B	222	ASN
1	B	307	ASN
1	B	314	ASN
1	B	343	GLN
1	B	352	GLN
1	B	367	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\|>2$
1	SEP	A	163	1	7,9,10	2.37	2 (28%)	8,12,14	2.82	3 (37%)
1	TPO	A	239	1	7,10,11	1.00	0	10,14,16	1.09	1 (10%)
1	SEP	B	163	1	7,9,10	2.06	1 (14%)	8,12,14	1.20	2 (25%)
1	TPO	B	239	1	7,10,11	0.68	0	10,14,16	1.70	3 (30%)

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
1	SEP	A	163	1	-	0/5/8/10	0/0/0/0
1	TPO	A	239	1	-	0/8/11/13	0/0/0/0
1	SEP	B	163	1	-	0/5/8/10	0/0/0/0
1	TPO	B	239	1	-	0/8/11/13	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	SEP	OG-CB	2.22	1.53	1.44
1	B	163	SEP	P-OG	4.80	1.73	1.59
1	A	163	SEP	P-OG	5.39	1.75	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	239	TPO	OG1-P-O1P	-2.79	100.81	107.48
1	B	239	TPO	O-C-CA	-2.59	118.61	125.69
1	A	239	TPO	O-C-CA	-2.07	120.03	125.69
1	B	163	SEP	OG-CB-CA	2.05	110.05	108.26
1	B	163	SEP	O3P-P-O2P	2.09	115.12	107.44
1	A	163	SEP	OG-P-O1P	2.18	112.58	107.08
1	B	239	TPO	C-CA-N	2.66	115.82	109.95
1	A	163	SEP	O3P-P-O2P	2.91	118.13	107.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	163	SEP	OG-CB-CA	6.70	114.10	108.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	163	SEP	1	0
1	A	239	TPO	2	0
1	B	239	TPO	1	0

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	$\#\|Z\| > 2$
2	GDP	A	500	3	24,30,30	1.49	3 (12%)	26,47,47	1.95	6 (23%)
2	GDP	B	500	3	24,30,30	1.25	2 (8%)	26,47,47	2.10	7 (26%)

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	GDP	A	500	3	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDP	B	500	3	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	GDP	C2'-C1'	-3.03	1.48	1.53
2	A	500	GDP	C5-C4	2.47	1.46	1.40
2	B	500	GDP	C5-C4	3.06	1.47	1.40
2	A	500	GDP	O4'-C1'	3.13	1.45	1.41
2	A	500	GDP	C6-C5	4.50	1.50	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	GDP	C5-C6-N1	-5.13	116.81	123.52
2	B	500	GDP	C5-C6-N1	-4.00	118.29	123.52
2	B	500	GDP	C6-C5-C4	-3.59	116.75	120.86
2	B	500	GDP	N3-C2-N1	-3.56	122.72	127.56
2	A	500	GDP	C6-C5-C4	-3.26	117.13	120.86
2	A	500	GDP	N3-C2-N1	-2.79	123.76	127.56
2	B	500	GDP	C1'-N9-C4	-2.56	123.95	126.81
2	A	500	GDP	O3'-C3'-C4'	-2.19	104.46	111.01
2	B	500	GDP	O3'-C3'-C2'	-2.05	105.22	111.86
2	A	500	GDP	C4'-O4'-C1'	2.46	112.25	109.64
2	B	500	GDP	O3B-PB-O2B	3.96	121.97	107.44
2	A	500	GDP	C6-N1-C2	4.86	121.58	115.88
2	B	500	GDP	C6-N1-C2	6.20	123.15	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	GDP	3	0

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	449/463 (96%)	0.05	19 (4%) 40 39	30, 66, 113, 149	0
1	B	440/463 (95%)	-0.23	6 (1%) 78 77	29, 49, 86, 111	0
All	All	889/926 (96%)	-0.09	25 (2%) 56 57	29, 55, 107, 149	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	SER	4.0
1	A	430	ARG	3.6
1	B	258	GLY	3.4
1	A	258	GLY	3.4
1	A	255	LYS	3.3
1	A	51	LYS	3.2
1	A	447	GLY	3.2
1	A	257	GLY	2.8
1	A	296	HIS	2.7
1	B	445	SER	2.7
1	B	430	ARG	2.6
1	A	326	CYS	2.5
1	A	297	GLU	2.4
1	A	445	SER	2.4
1	A	259	ILE	2.4
1	A	222	ASN	2.4
1	A	319	ASP	2.3
1	B	113	VAL	2.3
1	A	350	PRO	2.2
1	A	54	PHE	2.2
1	A	444	LYS	2.1
1	B	130	ASN	2.1
1	A	4	GLU	2.1
1	A	450	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	191	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	TPO	A	239	11/12	0.84	0.21	-	117,125,150,152	0
1	SEP	A	163	10/11	0.84	0.18	-	41,49,76,84	0
1	TPO	B	239	11/12	0.85	0.23	-	75,88,129,139	0
1	SEP	B	163	10/11	0.84	0.15	-	42,69,83,95	0

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	GDP	B	500	28/28	0.98	0.12	-0.64	30,44,59,66	0
2	GDP	A	500	28/28	0.98	0.11	-1.04	31,41,49,49	0
3	MG	A	501	1/1	0.86	0.13	-	49,49,49,49	0
3	MG	B	501	1/1	0.74	0.22	-	53,53,53,53	0

6.5 Other polymers (i)

There are no such residues in this entry.