



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:03 am BST

PDB ID : 5VBN
Title : Crystal Structure of human DNA polymerase epsilon B-subunit in complex with C-terminal domain of catalytic subunit
Authors : Baranovskiy, A.G.; Gu, J.; Suwa, Y.; Babayeva, N.D.; Tahirov, T.H.
Deposited on : 2017-03-29
Resolution : 2.35 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

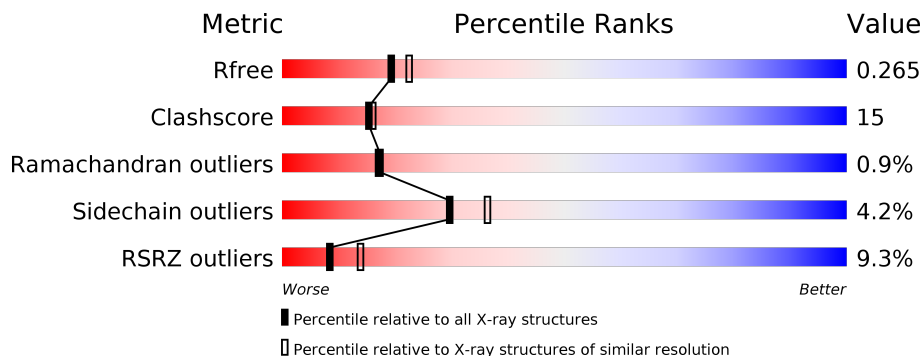
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 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	527	 4% 58% 20% 19%
1	E	527	 5% 60% 19% 19%
2	B	145	 14% 53% 30% 14%
2	F	145	 23% 43% 41% 14%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9058 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.

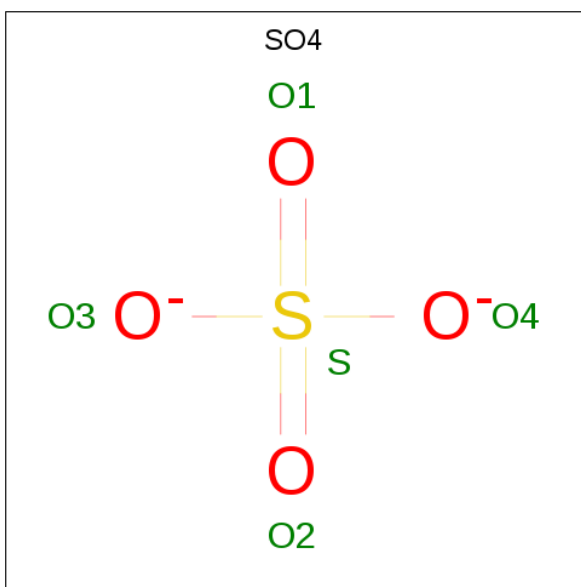
- Molecule 1 is a protein called DNA polymerase epsilon subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	427	Total 3425	C 2219	N 565	O 624	S 17	0	0	0
1	E	427	Total 3425	C 2219	N 565	O 624	S 17	0	0	0

- Molecule 2 is a protein called DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	125	Total 991	C 631	N 161	O 184	S 15	0	0	0
2	F	125	Total 991	C 631	N 161	O 184	S 15	0	0	0

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



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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Zn	0	0
			2	2		
4	F	2	Total	Zn	0	0
			2	2		

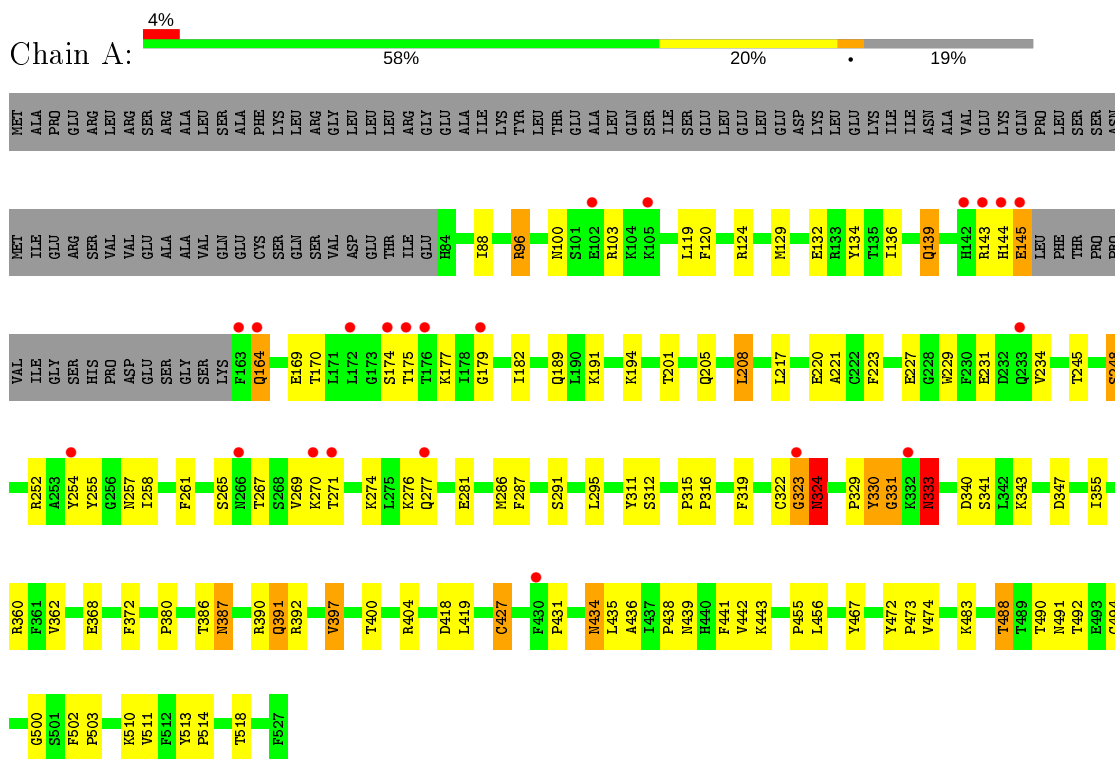
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total	O	0	0
			108	108		
5	B	6	Total	O	0	0
			6	6		
5	E	94	Total	O	0	0
			94	94		
5	F	4	Total	O	0	0
			4	4		

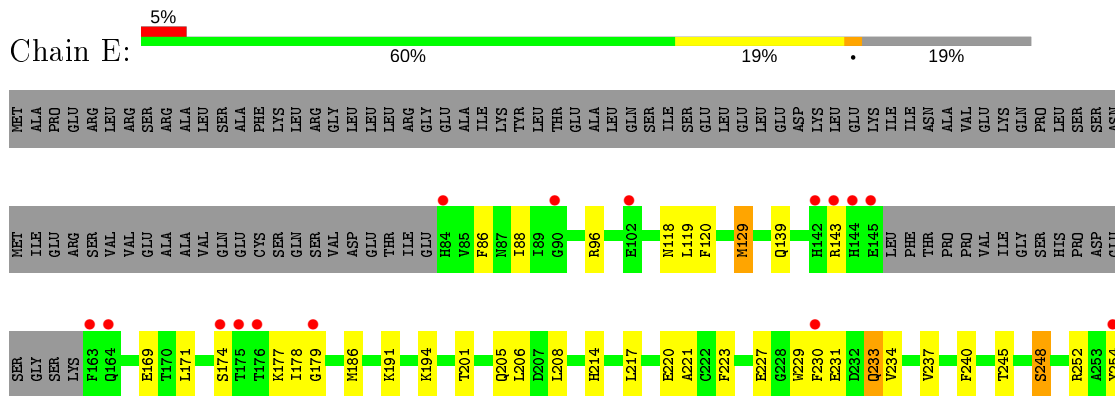
3 Residue-property plots

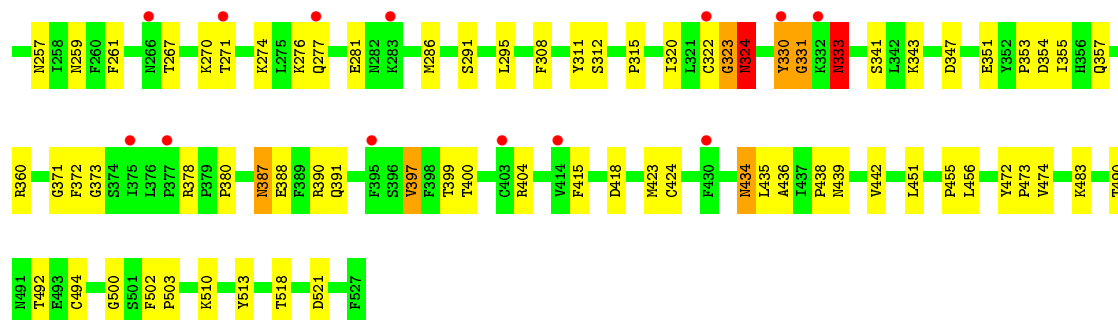
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: DNA polymerase epsilon subunit 2

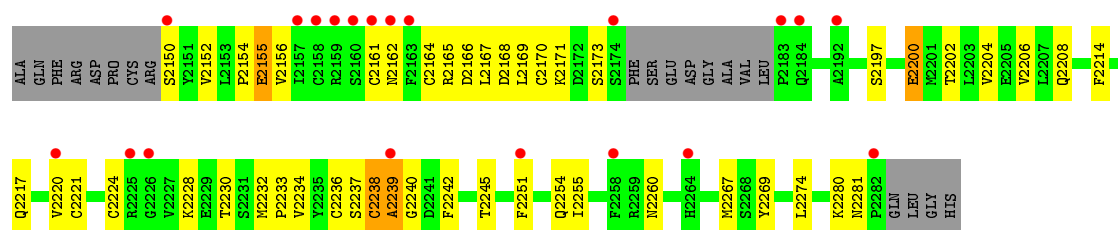


- Molecule 1: DNA polymerase epsilon subunit 2

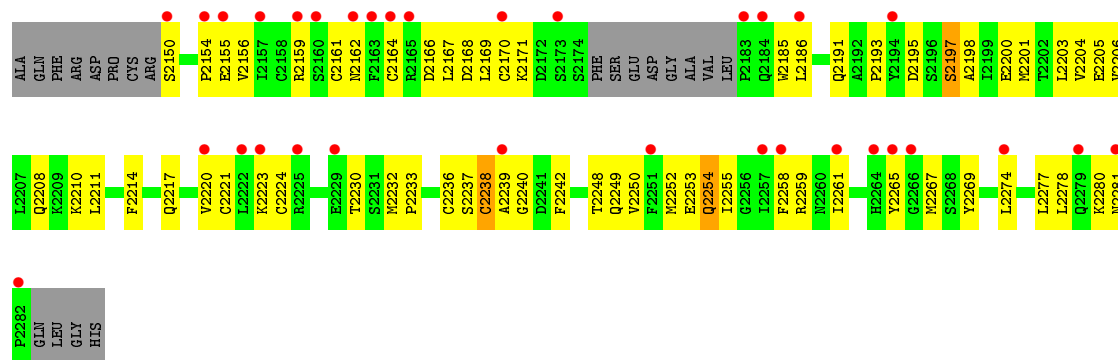
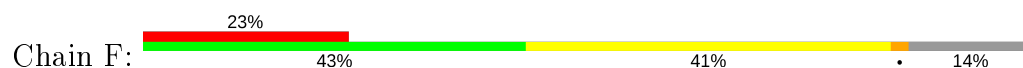




- Molecule 2: DNA polymerase epsilon catalytic subunit A



- Molecule 2: DNA polymerase epsilon catalytic subunit A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	92.26Å 201.46Å 78.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.75 – 2.35 39.75 – 2.33	Depositor EDS
% Data completeness (in resolution range)	94.7 (39.75-2.35) 93.9 (39.75-2.33)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.34Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.264 0.228 , 0.265	Depositor DCC
R_{free} test set	3117 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtrriage
Anisotropy	0.592	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9058	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.9667e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.48	0/3526	0.70	3/4794 (0.1%)
1	E	0.46	0/3526	0.69	3/4794 (0.1%)
2	B	0.39	0/1010	0.68	1/1365 (0.1%)
2	F	0.40	0/1010	0.68	1/1365 (0.1%)
All	All	0.45	0/9072	0.69	8/12318 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	331	GLY	N-CA-C	6.93	130.44	113.10
1	A	331	GLY	N-CA-C	6.91	130.38	113.10
1	E	324	ASN	N-CA-C	-6.37	93.79	111.00
1	A	324	ASN	N-CA-C	-6.31	93.95	111.00
1	E	323	GLY	N-CA-C	5.65	127.22	113.10
1	A	323	GLY	N-CA-C	5.62	127.16	113.10
2	F	2239	ALA	N-CA-C	-5.09	97.25	111.00
2	B	2239	ALA	N-CA-C	-5.00	97.50	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	3425	0	3361	100	0
1	E	3425	0	3361	86	0
2	B	991	0	977	39	0
2	F	991	0	977	52	0
3	A	5	0	0	0	0
3	E	5	0	0	0	0
4	B	2	0	0	0	0
4	F	2	0	0	0	0
5	A	108	0	0	4	0
5	B	6	0	0	0	0
5	E	94	0	0	2	0
5	F	4	0	0	0	0
All	All	9058	0	8676	261	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 15.

All (261) 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:513:TYR:HB2	1:A:518:THR:HG22	1.55	0.85
1:E:513:TYR:HB2	1:E:518:THR:HG22	1.57	0.84
2:B:2167:LEU:HD22	2:B:2169:LEU:HD23	1.58	0.84
1:A:488:THR:HG22	1:A:510:LYS:HZ1	1.41	0.83
1:E:343:LYS:HE3	1:E:388:GLU:OE1	1.80	0.81
2:F:2255:ILE:HG23	2:F:2274:LEU:HD22	1.61	0.80
2:B:2200:GLU:OE1	2:B:2269:TYR:HB3	1.84	0.78
2:F:2236:CYS:SG	2:F:2237:SER:N	2.57	0.78
1:E:418:ASP:OD1	1:E:483:LYS:HE3	1.85	0.77
2:B:2238:CYS:HB2	2:B:2240:GLY:H	1.51	0.76
1:A:139:GLN:HG2	1:A:143:ARG:HH12	1.52	0.75
2:B:2155:GLU:HB3	2:B:2164:CYS:SG	2.26	0.75
2:F:2155:GLU:HB3	2:F:2164:CYS:SG	2.27	0.74
1:A:488:THR:HG22	1:A:510:LYS:NZ	2.03	0.74
1:A:513:TYR:HB2	1:A:518:THR:CG2	2.18	0.74
2:F:2238:CYS:HB2	2:F:2240:GLY:H	1.52	0.74
1:E:434:ASN:HD22	1:E:434:ASN:C	1.91	0.73
1:E:143:ARG:NH1	1:E:254:TYR:HB3	2.04	0.72
1:E:119:LEU:HB2	2:F:2281:ASN:HD21	1.55	0.72
1:E:86:PHE:CE1	1:E:360:ARG:HD3	2.26	0.70
1:A:144:HIS:O	1:A:145:GLU:HG3	1.91	0.70
1:A:434:ASN:C	1:A:434:ASN:HD22	1.93	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:502:PHE:HB3	1:E:503:PRO:HD3	1.73	0.69
1:A:217:LEU:HD22	1:A:427:CYS:SG	2.33	0.69
2:F:2186:LEU:HD22	2:F:2191:GLN:O	1.92	0.69
2:B:2154:PRO:HA	2:B:2166:ASP:OD1	1.93	0.68
1:A:277:GLN:O	1:A:281:GLU:HG3	1.93	0.68
1:E:513:TYR:HB2	1:E:518:THR:CG2	2.23	0.68
2:B:2255:ILE:HG23	2:B:2274:LEU:HD22	1.74	0.68
1:E:277:GLN:O	1:E:281:GLU:HG3	1.94	0.67
2:F:2167:LEU:HD22	2:F:2169:LEU:HD23	1.74	0.67
2:F:2186:LEU:HD23	2:F:2193:PRO:HA	1.77	0.67
1:A:502:PHE:HB3	1:A:503:PRO:HD3	1.77	0.66
2:F:2150:SER:HB3	2:F:2171:LYS:HZ3	1.60	0.65
1:E:119:LEU:HG	2:F:2280:LYS:HB3	1.76	0.65
1:A:418:ASP:CG	1:A:483:LYS:HE3	2.16	0.65
1:A:380:PRO:HD3	1:A:400:THR:HG22	1.79	0.65
2:F:2200:GLU:CG	2:F:2267:MET:HB3	2.28	0.64
1:E:143:ARG:HH12	1:E:254:TYR:HB3	1.61	0.64
1:E:418:ASP:CG	1:E:483:LYS:HE3	2.18	0.64
1:E:245:THR:HG22	1:E:492:THR:HG21	1.78	0.63
1:A:119:LEU:HG	2:B:2280:LYS:HB3	1.80	0.63
1:A:286:MET:HE3	1:A:511:VAL:HG13	1.80	0.63
2:F:2159:ARG:NH2	2:F:2198:ALA:HB2	2.14	0.62
1:E:286:MET:HE1	1:E:311:TYR:CE2	2.34	0.61
1:A:271:THR:O	1:A:271:THR:HG22	2.01	0.60
1:E:333:ASN:N	1:E:333:ASN:HD22	2.00	0.58
1:A:119:LEU:HB2	2:B:2281:ASN:HD21	1.68	0.58
2:B:2236:CYS:SG	2:B:2237:SER:N	2.76	0.58
1:E:129:MET:SD	1:E:456:LEU:HD21	2.44	0.58
1:E:86:PHE:HE1	1:E:360:ARG:HD3	1.69	0.58
2:F:2200:GLU:CD	2:F:2267:MET:HB3	2.24	0.58
1:E:353:PRO:O	1:E:357:GLN:HG3	2.04	0.58
2:B:2150:SER:HA	2:B:2170:CYS:SG	2.43	0.58
2:B:2214:PHE:O	2:B:2217:GLN:HG2	2.04	0.57
1:A:169:GLU:HB3	1:A:201:THR:HB	1.86	0.57
2:F:2150:SER:HA	2:F:2170:CYS:HB2	1.87	0.57
1:E:387:ASN:OD1	1:E:390:ARG:NH2	2.38	0.57
2:F:2195:ASP:OD2	2:F:2197:SER:HB3	2.05	0.56
1:A:120:PHE:CD1	2:B:2281:ASN:ND2	2.74	0.56
1:A:139:GLN:CG	1:A:143:ARG:HH12	2.17	0.56
1:A:257:ASN:HB3	1:A:267:THR:HG23	1.86	0.56
1:E:387:ASN:HA	1:E:390:ARG:NH2	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:248:SER:HB2	1:E:252:ARG:NH2	2.21	0.56
2:B:2150:SER:HB2	2:B:2168:ASP:OD1	2.06	0.56
2:F:2150:SER:HB3	2:F:2171:LYS:NZ	2.20	0.56
1:A:286:MET:HE2	1:A:311:TYR:CZ	2.40	0.56
1:A:474:VAL:CG1	1:A:494:CYS:HB2	2.37	0.55
2:F:2161:CYS:O	2:F:2162:ASN:HB2	2.07	0.55
1:A:261:PHE:CZ	1:A:404:ARG:HB3	2.42	0.55
1:E:177:LYS:HD3	1:E:231:GLU:CD	2.27	0.55
2:F:2250:VAL:O	2:F:2254:GLN:NE2	2.40	0.55
1:E:271:THR:O	1:E:271:THR:HG22	2.07	0.55
1:E:387:ASN:HA	1:E:390:ARG:HH21	1.72	0.55
1:A:139:GLN:HG2	1:A:143:ARG:NH1	2.22	0.54
1:A:144:HIS:O	1:A:145:GLU:CG	2.56	0.54
2:B:2161:CYS:O	2:B:2162:ASN:HB2	2.07	0.54
1:E:436:ALA:HB3	1:E:439:ASN:HD22	1.72	0.54
1:A:315:PRO:HB3	1:A:355:ILE:HD13	1.90	0.54
1:E:474:VAL:CG1	1:E:494:CYS:HB2	2.38	0.54
1:E:333:ASN:HB2	5:E:782:HOH:O	2.06	0.54
1:A:132:GLU:O	1:A:136:ILE:HD13	2.08	0.53
1:A:100:ASN:OD1	1:A:103:ARG:N	2.36	0.53
1:A:286:MET:HE3	1:A:511:VAL:CG1	2.39	0.53
2:F:2200:GLU:O	2:F:2204:VAL:HG23	2.08	0.53
2:F:2249:GLN:O	2:F:2253:GLU:HG3	2.08	0.53
1:E:205:GLN:HG2	1:E:234:VAL:HG22	1.90	0.53
1:A:248:SER:HB2	1:A:252:ARG:NH2	2.24	0.52
1:E:323:GLY:O	1:E:324:ASN:HB2	2.09	0.52
1:A:177:LYS:HB2	1:A:231:GLU:OE2	2.10	0.52
1:A:286:MET:HE2	1:A:311:TYR:CE2	2.45	0.52
1:A:291:SER:HA	1:A:322:CYS:HB2	1.90	0.52
1:A:387:ASN:HA	1:A:390:ARG:NH2	2.23	0.52
1:E:434:ASN:HD22	1:E:435:LEU:N	2.08	0.52
1:E:220:GLU:O	1:E:455:PRO:HD3	2.09	0.52
1:E:415:PHE:CD1	1:E:451:LEU:HD22	2.44	0.52
1:E:261:PHE:CZ	1:E:404:ARG:HB3	2.45	0.52
1:A:434:ASN:ND2	1:A:434:ASN:C	2.62	0.52
2:F:2230:THR:OG1	2:F:2233:PRO:HG3	2.08	0.52
1:A:269:VAL:HG22	5:A:713:HOH:O	2.09	0.52
2:B:2150:SER:HA	2:B:2170:CYS:HB2	1.92	0.52
1:A:191:LYS:HB2	1:A:194:LYS:HD2	1.92	0.51
2:B:2230:THR:OG1	2:B:2233:PRO:HG3	2.09	0.51
1:E:217:LEU:HD23	1:E:423:MET:HE2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:ALA:HB3	1:A:439:ASN:HD22	1.76	0.51
1:A:274:LYS:O	1:A:277:GLN:HB3	2.10	0.51
2:B:2251:PHE:O	2:B:2254:GLN:HB2	2.10	0.51
1:E:120:PHE:CD1	2:F:2281:ASN:ND2	2.79	0.51
1:E:330:TYR:CD2	1:E:330:TYR:N	2.77	0.51
1:A:208:LEU:CD2	1:A:208:LEU:H	2.24	0.51
1:A:323:GLY:O	1:A:324:ASN:HB2	2.11	0.51
1:A:333:ASN:HD22	1:A:333:ASN:N	2.08	0.51
1:A:220:GLU:O	1:A:221:ALA:HB3	2.11	0.51
1:E:220:GLU:O	1:E:221:ALA:HB3	2.11	0.51
2:F:2150:SER:HA	2:F:2170:CYS:SG	2.51	0.51
1:E:88:ILE:CD1	1:E:397:VAL:HG11	2.41	0.51
2:B:2204:VAL:O	2:B:2208:GLN:HG3	2.11	0.50
1:A:270:LYS:HG3	5:A:731:HOH:O	2.10	0.50
2:B:2200:GLU:CG	2:B:2267:MET:HB3	2.42	0.50
2:F:2206:VAL:O	2:F:2210:LYS:HG3	2.11	0.50
1:A:419:LEU:HD23	1:A:441:PHE:HZ	1.77	0.50
1:E:434:ASN:ND2	1:E:434:ASN:C	2.62	0.50
1:A:329:PRO:HG2	1:A:368:GLU:OE1	2.12	0.50
2:B:2150:SER:HB3	2:B:2171:LYS:NZ	2.26	0.50
1:A:434:ASN:HD22	1:A:435:LEU:N	2.10	0.50
1:E:308:PHE:O	1:E:355:ILE:HD11	2.12	0.50
2:F:2220:VAL:O	2:F:2242:PHE:HA	2.12	0.50
2:F:2261:ILE:O	2:F:2265:TYR:HD1	1.94	0.50
1:A:330:TYR:CD1	1:A:330:TYR:N	2.80	0.50
1:E:312:SER:O	1:E:315:PRO:HD3	2.12	0.50
2:B:2220:VAL:HG23	2:B:2245:THR:CG2	2.42	0.49
1:A:340:ASP:HA	1:A:343:LYS:HE3	1.93	0.49
1:E:291:SER:HA	1:E:322:CYS:HB2	1.94	0.49
1:E:177:LYS:HG3	1:E:231:GLU:HB2	1.95	0.49
2:B:2228:LYS:HE3	2:B:2233:PRO:HG2	1.94	0.49
1:A:179:GLY:O	1:A:229:TRP:HB3	2.14	0.48
1:E:380:PRO:HD3	1:E:400:THR:HG22	1.95	0.48
1:A:205:GLN:HG2	1:A:234:VAL:HG22	1.95	0.48
1:E:333:ASN:ND2	1:E:333:ASN:N	2.60	0.48
2:F:2154:PRO:HA	2:F:2166:ASP:OD1	2.12	0.48
1:A:217:LEU:HD23	1:A:431:PRO:HG3	1.95	0.48
1:A:120:PHE:HD1	2:B:2281:ASN:ND2	2.11	0.48
2:F:2232:MET:N	2:F:2233:PRO:HD2	2.29	0.48
1:E:186:MET:HB2	1:E:223:PHE:CE2	2.48	0.48
2:F:2150:SER:HB2	2:F:2168:ASP:OD2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2255:ILE:HG23	2:F:2274:LEU:CD2	2.40	0.48
1:A:372:PHE:CD1	2:B:2208:GLN:HG2	2.49	0.48
1:E:492:THR:O	1:E:492:THR:HG22	2.13	0.48
1:E:438:PRO:O	1:E:442:VAL:HG23	2.14	0.47
2:B:2167:LEU:CD2	2:B:2169:LEU:HD23	2.38	0.47
1:E:373:GLY:HA2	1:E:378:ARG:HD2	1.96	0.47
2:F:2159:ARG:NH1	2:F:2195:ASP:OD1	2.47	0.47
1:A:438:PRO:O	1:A:442:VAL:HG23	2.14	0.47
1:E:320:ILE:HD12	1:E:320:ILE:N	2.29	0.47
1:A:347:ASP:OD1	1:A:392:ARG:NH1	2.42	0.47
1:A:88:ILE:HD12	1:A:397:VAL:HG11	1.96	0.47
1:A:324:ASN:HD21	1:A:368:GLU:HG3	1.79	0.47
1:A:372:PHE:CE1	2:B:2208:GLN:HG2	2.50	0.47
2:B:2220:VAL:O	2:B:2242:PHE:HA	2.15	0.47
1:A:217:LEU:HD23	1:A:431:PRO:CG	2.45	0.47
1:E:257:ASN:HB3	1:E:267:THR:CG2	2.45	0.47
1:E:399:THR:OG1	1:E:400:THR:N	2.48	0.47
1:A:490:THR:O	1:A:490:THR:HG23	2.15	0.46
1:E:354:ASP:HB2	5:E:759:HOH:O	2.15	0.46
1:A:443:LYS:HG2	1:A:491:ASN:ND2	2.30	0.46
1:E:169:GLU:HB3	1:E:201:THR:HB	1.96	0.46
1:E:252:ARG:CZ	1:E:270:LYS:HG2	2.45	0.46
2:F:2259:ARG:HA	2:F:2274:LEU:HD13	1.97	0.46
1:A:96:ARG:NH2	1:A:132:GLU:OE1	2.46	0.46
1:E:206:LEU:HD22	1:E:237:VAL:CG2	2.46	0.46
1:E:371:GLY:O	2:F:2208:GLN:NE2	2.48	0.46
1:A:258:ILE:HD12	1:A:258:ILE:N	2.31	0.46
1:A:287:PHE:HE1	1:A:514:PRO:HG3	1.80	0.46
1:A:360:ARG:HD3	5:A:737:HOH:O	2.14	0.46
2:B:2202:THR:O	2:B:2206:VAL:HG23	2.15	0.46
1:A:265:SER:OG	1:A:267:THR:O	2.28	0.46
1:A:333:ASN:ND2	1:A:333:ASN:N	2.63	0.46
1:E:387:ASN:CA	1:E:390:ARG:HH21	2.28	0.46
2:F:2150:SER:HA	2:F:2170:CYS:CB	2.45	0.46
2:F:2186:LEU:HD23	2:F:2193:PRO:CA	2.44	0.46
1:E:415:PHE:HD1	1:E:451:LEU:HD22	1.82	0.45
1:E:415:PHE:CE1	1:E:451:LEU:HB3	2.52	0.45
2:B:2232:MET:N	2:B:2233:PRO:HD2	2.31	0.45
1:A:245:THR:HG22	1:A:492:THR:HG21	1.97	0.45
1:E:286:MET:HE3	1:E:311:TYR:OH	2.15	0.45
2:F:2200:GLU:OE1	2:F:2269:TYR:HB3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:472:TYR:HA	1:E:473:PRO:C	2.37	0.45
1:A:255:TYR:O	1:A:258:ILE:HD13	2.17	0.45
1:A:295:LEU:HB2	1:A:341:SER:HB3	1.98	0.45
1:A:96:ARG:HG3	1:A:467:TYR:CE2	2.51	0.45
1:E:143:ARG:NH1	1:E:254:TYR:CB	2.78	0.45
1:A:220:GLU:O	1:A:455:PRO:HD3	2.16	0.45
1:E:230:PHE:CZ	1:E:233:GLN:HA	2.52	0.45
2:B:2238:CYS:HB2	2:B:2239:ALA:H	1.29	0.44
1:E:510:LYS:HD3	1:E:521:ASP:OD1	2.17	0.44
2:B:2156:VAL:HG21	2:B:2167:LEU:HD12	1.99	0.44
2:B:2150:SER:HA	2:B:2170:CYS:CB	2.47	0.44
1:A:316:PRO:HG2	1:A:319:PHE:CE1	2.53	0.44
1:E:347:ASP:O	1:E:351:GLU:HG3	2.18	0.44
1:E:274:LYS:O	1:E:277:GLN:HB3	2.17	0.44
2:F:2203:LEU:HD22	2:F:2258:PHE:HE1	1.82	0.44
2:F:2156:VAL:HG21	2:F:2167:LEU:HD12	2.00	0.44
1:A:391:GLN:HE21	1:A:391:GLN:HB3	1.62	0.44
1:E:257:ASN:HB3	1:E:267:THR:HG23	1.99	0.44
1:A:191:LYS:HB2	1:A:194:LYS:HB2	2.00	0.44
1:A:88:ILE:HD13	1:A:362:VAL:HG22	2.00	0.44
1:A:124:ARG:NH1	2:B:2234:VAL:HG11	2.32	0.44
1:E:490:THR:O	1:E:490:THR:HG23	2.18	0.43
1:A:312:SER:O	1:A:315:PRO:HD3	2.18	0.43
1:E:286:MET:CE	1:E:311:TYR:CE2	3.01	0.43
1:A:145:GLU:CD	1:A:145:GLU:C	2.76	0.43
1:E:343:LYS:HE3	1:E:388:GLU:CD	2.38	0.43
2:F:2201:MET:O	2:F:2205:GLU:HG3	2.17	0.43
2:F:2248:THR:O	2:F:2252:MET:HG2	2.18	0.43
1:A:343:LYS:HA	5:A:778:HOH:O	2.16	0.43
1:A:472:TYR:HA	1:A:473:PRO:C	2.39	0.43
1:A:88:ILE:CD1	1:A:397:VAL:HG11	2.48	0.43
1:A:96:ARG:HG2	1:A:96:ARG:HH11	1.84	0.43
1:E:119:LEU:HB2	2:F:2281:ASN:ND2	2.27	0.43
1:E:179:GLY:O	1:E:229:TRP:HB3	2.19	0.43
1:E:191:LYS:HB2	1:E:194:LYS:HB2	2.00	0.43
1:A:119:LEU:HG	2:B:2280:LYS:CB	2.48	0.43
1:A:129:MET:SD	1:A:456:LEU:HD21	2.59	0.43
1:A:143:ARG:HD2	1:A:254:TYR:CE2	2.54	0.42
1:A:492:THR:O	1:A:492:THR:HG22	2.17	0.42
2:F:2204:VAL:O	2:F:2208:GLN:HG3	2.18	0.42
1:A:189:GLN:HG2	1:A:191:LYS:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ASP:O	1:A:343:LYS:HB2	2.19	0.42
1:A:169:GLU:HG2	1:A:170:THR:N	2.35	0.42
1:E:208:LEU:C	1:E:208:LEU:HD12	2.39	0.42
1:A:164:GLN:HE21	1:A:164:GLN:HB3	1.60	0.42
1:A:386:THR:O	1:A:390:ARG:HD3	2.20	0.42
2:B:2152:VAL:HA	2:B:2167:LEU:O	2.19	0.42
1:E:217:LEU:HD23	1:E:423:MET:CE	2.50	0.42
2:F:2214:PHE:O	2:F:2217:GLN:HG2	2.19	0.42
2:F:2223:LYS:HD2	2:F:2238:CYS:HB3	2.02	0.42
2:B:2152:VAL:CG2	2:B:2166:ASP:HB3	2.50	0.41
2:F:2221:CYS:HB3	2:F:2224:CYS:O	2.19	0.41
1:A:488:THR:CG2	1:A:510:LYS:HZ1	2.19	0.41
1:A:418:ASP:OD1	1:A:483:LYS:HE3	2.20	0.41
2:F:2211:LEU:HD22	2:F:2277:LEU:HD11	2.02	0.41
1:E:171:LEU:HD22	1:E:178:ILE:HD12	2.03	0.41
2:F:2200:GLU:HA	2:F:2267:MET:HE1	2.02	0.41
2:B:2221:CYS:HB3	2:B:2224:CYS:O	2.21	0.41
1:E:88:ILE:HD12	1:E:397:VAL:HG11	2.02	0.41
1:E:118:ASN:HB3	2:F:2281:ASN:OD1	2.21	0.41
1:A:295:LEU:CB	1:A:341:SER:HB3	2.51	0.41
1:E:295:LEU:HB2	1:E:341:SER:HB3	2.03	0.41
1:E:88:ILE:HD13	1:E:397:VAL:HG11	2.03	0.41
2:B:2167:LEU:HD23	2:B:2167:LEU:C	2.41	0.41
1:E:214:HIS:HD2	1:E:240:PHE:O	2.03	0.41
2:F:2185:TRP:CH2	2:F:2265:TYR:CD2	3.09	0.40
2:F:2169:LEU:HD11	2:F:2203:LEU:HD21	2.04	0.40
1:E:120:PHE:HD1	2:F:2281:ASN:ND2	2.19	0.40
1:A:134:TYR:HB2	1:A:223:PHE:CE2	2.56	0.40
1:E:372:PHE:CD1	2:F:2208:GLN:HG2	2.56	0.40
1:A:274:LYS:HE2	1:A:274:LYS:HB3	1.87	0.40
2:B:2150:SER:HB3	2:B:2171:LYS:HZ2	1.87	0.40
1:A:419:LEU:HD23	1:A:441:PHE:CZ	2.55	0.40
1:A:291:SER:HB3	1:A:500:GLY:O	2.22	0.40
1:E:291:SER:HB3	1:E:500:GLY:O	2.21	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	423/527 (80%)	401 (95%)	18 (4%)	4 (1%)	17	17
1	E	423/527 (80%)	402 (95%)	17 (4%)	4 (1%)	17	17
2	B	121/145 (83%)	111 (92%)	9 (7%)	1 (1%)	19	20
2	F	121/145 (83%)	111 (92%)	9 (7%)	1 (1%)	19	20
All	All	1088/1344 (81%)	1025 (94%)	53 (5%)	10 (1%)	17	17

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	ASN
2	B	2238	CYS
1	E	333	ASN
2	F	2238	CYS
1	A	174	SER
1	A	331	GLY
1	E	174	SER
1	E	331	GLY
1	A	324	ASN
1	E	324	ASN

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	383/471 (81%)	365 (95%)	18 (5%)	26	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	383/471 (81%)	368 (96%)	15 (4%)	32	40
2	B	115/131 (88%)	109 (95%)	6 (5%)	23	27
2	F	115/131 (88%)	112 (97%)	3 (3%)	46	56
All	All	996/1204 (83%)	954 (96%)	42 (4%)	30	36

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ARG
1	A	139	GLN
1	A	145	GLU
1	A	164	GLN
1	A	175	THR
1	A	182	ILE
1	A	208	LEU
1	A	227	GLU
1	A	248	SER
1	A	276	LYS
1	A	330	TYR
1	A	333	ASN
1	A	387	ASN
1	A	391	GLN
1	A	397	VAL
1	A	427	CYS
1	A	434	ASN
1	A	488	THR
2	B	2155	GLU
2	B	2165	ARG
2	B	2173	SER
2	B	2197	SER
2	B	2200	GLU
2	B	2260	ASN
1	E	96	ARG
1	E	129	MET
1	E	139	GLN
1	E	227	GLU
1	E	233	GLN
1	E	248	SER
1	E	259	ASN
1	E	276	LYS
1	E	330	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	333	ASN
1	E	387	ASN
1	E	391	GLN
1	E	397	VAL
1	E	424	CYS
1	E	434	ASN
2	F	2197	SER
2	F	2254	GLN
2	F	2278	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	GLN
1	A	333	ASN
1	A	334	GLN
1	A	357	GLN
1	A	391	GLN
1	A	434	ASN
1	A	439	ASN
2	B	2184	GLN
2	B	2208	GLN
2	B	2263	GLN
1	E	139	GLN
1	E	214	HIS
1	E	259	ASN
1	E	297	GLN
1	E	333	ASN
1	E	334	GLN
1	E	357	GLN
1	E	391	GLN
1	E	410	GLN
1	E	426	ASN
1	E	434	ASN
1	E	439	ASN
2	F	2184	GLN
2	F	2208	GLN
2	F	2254	GLN
2	F	2263	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	601	-	4,4,4	0.30	0	6,6,6	0.20	0
3	SO4	E	601	-	4,4,4	0.21	0	6,6,6	0.11	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.

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

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	427/527 (81%)	0.30	22 (5%) 27 39	21, 38, 64, 80	0
1	E	427/527 (81%)	0.42	28 (6%) 18 26	22, 39, 67, 80	0
2	B	125/145 (86%)	1.00	20 (16%) 1 3	41, 58, 68, 71	0
2	F	125/145 (86%)	1.31	33 (26%) 0 0	42, 62, 72, 77	0
All	All	1104/1344 (82%)	0.54	103 (9%) 8 14	21, 44, 68, 80	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	332	LYS	6.3
2	F	2258	PHE	6.2
1	E	144	HIS	5.4
1	A	332	LYS	5.4
1	E	175	THR	5.3
2	F	2261	ILE	5.2
1	A	163	PHE	5.0
2	F	2159	ARG	4.9
2	F	2160	SER	4.9
2	B	2225	ARG	4.9
2	B	2157	ILE	4.8
2	F	2225	ARG	4.7
1	E	142	HIS	4.5
2	F	2163	PHE	4.5
2	B	2162	ASN	4.1
1	A	175	THR	4.1
1	A	254	TYR	4.0
2	B	2239	ALA	4.0
2	F	2162	ASN	4.0
2	F	2184	GLN	3.9
2	B	2192	ALA	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	2170	CYS	3.9
2	F	2150	SER	3.8
2	F	2264	HIS	3.7
2	F	2164	CYS	3.7
1	A	430	PHE	3.7
2	B	2163	PHE	3.6
2	B	2174	SER	3.5
2	B	2150	SER	3.5
2	B	2258	PHE	3.5
2	F	2220	VAL	3.5
2	F	2223	LYS	3.4
1	A	145	GLU	3.4
2	F	2257	ILE	3.4
2	F	2183	PRO	3.3
2	B	2220	VAL	3.3
2	F	2165	ARG	3.3
1	E	266	ASN	3.1
1	E	143	ARG	3.1
1	E	271	THR	3.1
1	A	270	LYS	3.0
2	B	2160	SER	3.0
1	E	254	TYR	3.0
2	F	2282	PRO	3.0
2	B	2184	GLN	3.0
1	E	176	THR	3.0
1	A	271	THR	2.9
1	A	144	HIS	2.9
2	B	2251	PHE	2.9
1	E	102	GLU	2.8
1	A	323	GLY	2.8
1	E	163	PHE	2.8
1	A	102	GLU	2.8
2	F	2239	ALA	2.8
1	A	172	LEU	2.8
1	A	174	SER	2.8
2	B	2159	ARG	2.7
1	E	395	PHE	2.7
2	F	2266	GLY	2.7
2	B	2183	PRO	2.7
2	B	2282	PRO	2.7
2	B	2161	CYS	2.6
1	A	179	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	174	SER	2.6
1	E	283	LYS	2.6
1	A	142	HIS	2.6
2	F	2265	TYR	2.5
2	F	2154	PRO	2.5
2	B	2226	GLY	2.5
2	F	2222	LEU	2.5
1	E	145	GLU	2.3
2	F	2155	GLU	2.3
1	E	179	GLY	2.3
1	E	164	GLN	2.3
1	E	90	GLY	2.3
1	A	143	ARG	2.3
1	E	330	TYR	2.3
2	F	2194	TYR	2.3
1	A	266	ASN	2.3
2	F	2186	LEU	2.2
1	A	164	GLN	2.2
2	F	2173	SER	2.2
1	E	322	CYS	2.2
1	E	403	CYS	2.2
1	A	176	THR	2.2
2	F	2251	PHE	2.2
1	E	377	PRO	2.2
1	A	277	GLN	2.2
1	E	414	VAL	2.1
2	F	2281	ASN	2.1
2	F	2229	GLU	2.1
1	A	105	LYS	2.1
2	F	2279	GLN	2.1
1	E	84	HIS	2.1
1	E	230	PHE	2.1
1	A	233	GLN	2.0
1	E	430	PHE	2.0
1	E	375	ILE	2.0
2	F	2157	ILE	2.0
2	B	2264	HIS	2.0
2	B	2158	CYS	2.0
2	F	2274	LEU	2.0
1	E	277	GLN	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. 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(\AA^2)	Q<0.9
4	ZN	F	2301	1/1	0.90	0.05	62,62,62,62	0
4	ZN	B	2302	1/1	0.95	0.03	66,66,66,66	0
4	ZN	F	2302	1/1	0.96	0.04	66,66,66,66	0
3	SO4	A	601	5/5	0.97	0.13	62,63,64,64	0
3	SO4	E	601	5/5	0.98	0.12	60,62,63,64	0
4	ZN	B	2301	1/1	0.99	0.04	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.