Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:08 AM GMT

PDB ID	:	3HB0
Title	:	Structure of edeya2 complexed with bef3
Authors	:	Jung, S.K.; Jeong, D.G.; Ryu, S.E.; Kim, S.J.
Deposited on	:	2009-05-03
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:

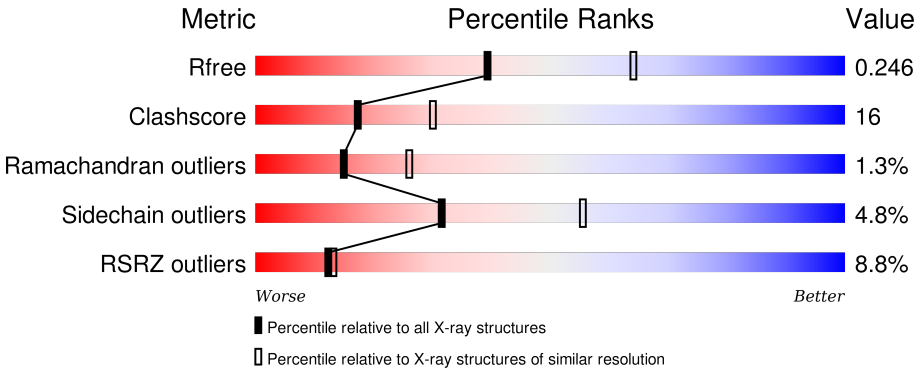
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	274	2% 67% 26% • 5%
1	B	274	12% 54% 35% •• 8%
1	C	274	12% 67% 25% • 5%
1	D	274	7% 65% 26% • 7%

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
3	MG	B	702	-	-	-	X
3	MG	D	704	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8448 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.

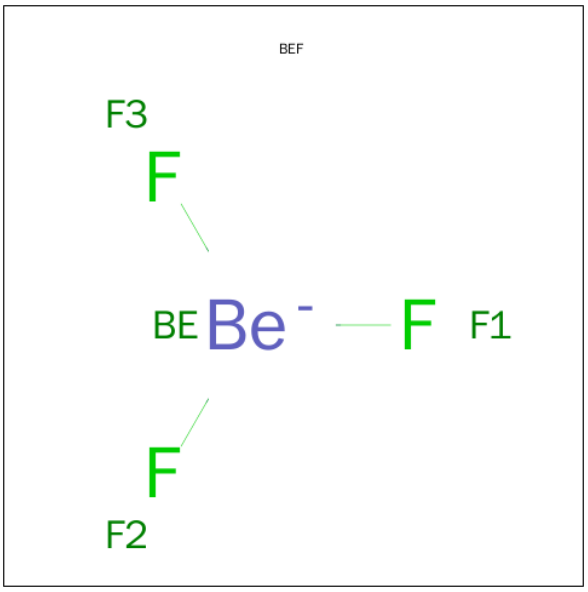
- Molecule 1 is a protein called Eyes absent homolog 2 (Drosophila).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			2088	1328	358	390	12			
1	B	253	Total	C	N	O	S	0	0	0
			2049	1305	350	383	11			
1	C	259	Total	C	N	O	S	0	0	0
			2088	1328	358	390	12			
1	D	256	Total	C	N	O	S	0	0	0
			2064	1314	353	386	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	SER	-	EXPRESSION TAG	UNP Q86U84
A	266	HIS	-	EXPRESSION TAG	UNP Q86U84
A	267	MET	-	EXPRESSION TAG	UNP Q86U84
A	268	GLU	-	EXPRESSION TAG	UNP Q86U84
B	265	SER	-	EXPRESSION TAG	UNP Q86U84
B	266	HIS	-	EXPRESSION TAG	UNP Q86U84
B	267	MET	-	EXPRESSION TAG	UNP Q86U84
B	268	GLU	-	EXPRESSION TAG	UNP Q86U84
C	265	SER	-	EXPRESSION TAG	UNP Q86U84
C	266	HIS	-	EXPRESSION TAG	UNP Q86U84
C	267	MET	-	EXPRESSION TAG	UNP Q86U84
C	268	GLU	-	EXPRESSION TAG	UNP Q86U84
D	265	SER	-	EXPRESSION TAG	UNP Q86U84
D	266	HIS	-	EXPRESSION TAG	UNP Q86U84
D	267	MET	-	EXPRESSION TAG	UNP Q86U84
D	268	GLU	-	EXPRESSION TAG	UNP Q86U84

- Molecule 2 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Be F 4 1 3	0	0
2	B	1	Total Be F 4 1 3	0	0
2	C	1	Total Be F 4 1 3	0	0
2	D	1	Total Be F 4 1 3	0	0

- 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
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	50	Total O 50 50	0	0

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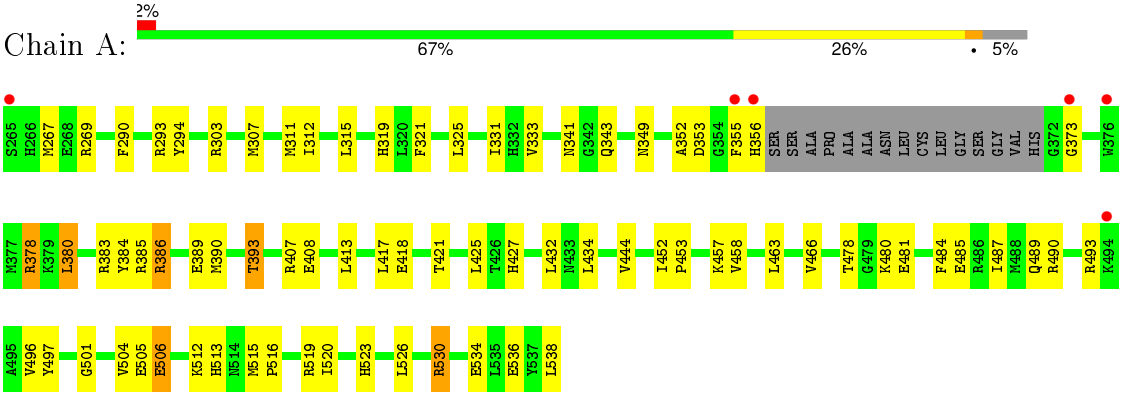
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	32	Total O 32 32	0	0
4	C	22	Total O 22 22	0	0
4	D	35	Total O 35 35	0	0

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.

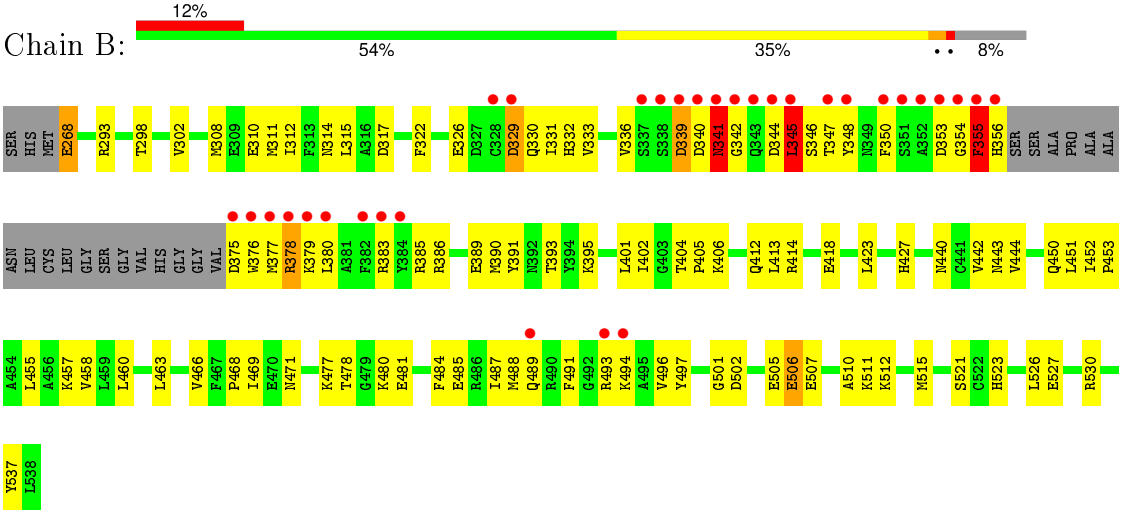
- Molecule 1: Eyes absent homolog 2 (Drosophila)

Chain A:



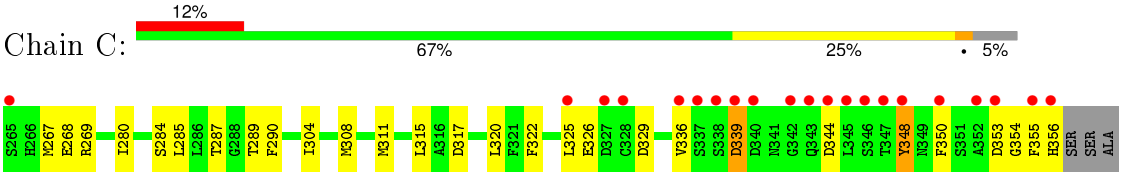
- Molecule 1: Eyes absent homolog 2 (Drosophila)

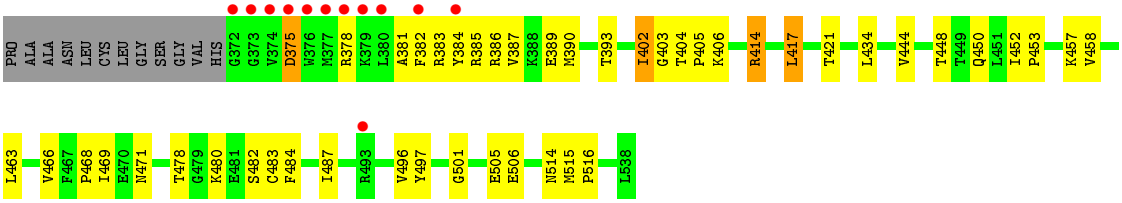
Chain B:



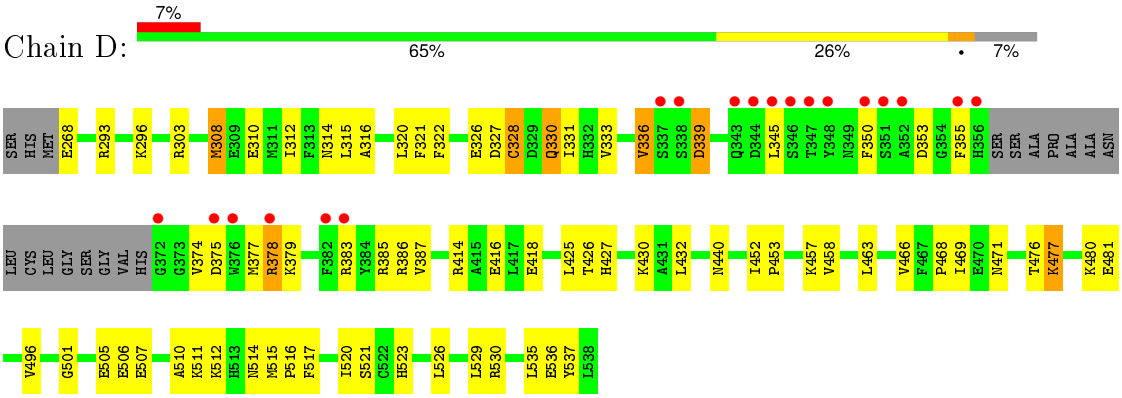
- Molecule 1: Eyes absent homolog 2 (Drosophila)

Chain C:





- Molecule 1: Eyes absent homolog 2 (Drosophila)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	184.00Å 184.00Å 119.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.50 46.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.3 (40.00-2.50) 93.3 (46.96-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.89 (at 2.51Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.224 , 0.254 0.219 , 0.246	Depositor DCC
R_{free} test set	3441 reflections (5.62%)	DCC
Wilson B-factor (Å^2)	42.5	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.8	EDS
Estimated twinning fraction	0.018 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 67585 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8448	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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: MG, BEF

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	0/2132	0.62	0/2882
1	B	0.38	0/2092	0.59	0/2829
1	C	0.37	0/2132	0.58	0/2882
1	D	0.39	0/2107	0.60	0/2849
All	All	0.38	0/8463	0.60	0/11442

There are no bond length outliers.

There are no bond angle outliers.

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	2088	0	2048	64	0
1	B	2049	0	2012	96	0
1	C	2088	0	2048	61	0
1	D	2064	0	2027	54	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	50	0	0	3	0
4	B	32	0	0	1	0
4	C	22	0	0	1	0
4	D	35	0	0	0	0
All	All	8448	0	8135	265	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 (265) 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:427:HIS:HD2	1:B:523:HIS:HE1	1.16	0.93
1:D:427:HIS:HD2	1:D:523:HIS:HE1	1.25	0.82
1:C:383:ARG:HH11	1:C:383:ARG:HG2	1.44	0.82
1:B:310:GLU:O	1:B:314:ASN:HB2	1.80	0.82
1:B:427:HIS:HD2	1:B:523:HIS:CE1	1.98	0.80
1:D:432:LEU:HB3	1:D:466:VAL:HG11	1.64	0.79
1:D:427:HIS:HD2	1:D:523:HIS:CE1	2.01	0.78
1:B:502:ASP:OD2	4:B:135:HOH:O	2.00	0.78
1:A:389:GLU:O	1:A:393:THR:HG23	1.83	0.77
1:B:339:ASP:HB3	1:B:377:MET:HB3	1.67	0.77
1:C:480:LYS:NZ	1:C:506:GLU:HG2	2.01	0.76
1:A:481:GLU:HG3	1:A:513:HIS:HE1	1.51	0.75
1:B:350:PHE:HB3	1:B:383:ARG:HH12	1.53	0.74
1:A:432:LEU:HB3	1:A:466:VAL:HG21	1.69	0.74
1:A:349:ASN:HD22	1:A:352:ALA:HB3	1.52	0.74
1:A:267:MET:HE3	1:D:496:VAL:HG11	1.69	0.72
1:A:349:ASN:ND2	1:A:352:ALA:HB3	2.04	0.72
1:A:444:VAL:HG11	1:A:487:ILE:HD13	1.71	0.72
1:B:333:VAL:HG21	1:B:469:ILE:HG12	1.72	0.71
1:B:336:VAL:HG11	1:B:380:LEU:HD12	1.72	0.71
1:C:402:ILE:HG23	1:C:406:LYS:HB2	1.72	0.71
1:A:530:ARG:HB3	1:A:530:ARG:HH11	1.55	0.71
1:A:269:ARG:NH2	1:D:537:TYR:O	2.24	0.70
1:C:315:LEU:HD12	1:C:402:ILE:HD11	1.72	0.70
1:B:496:VAL:HG11	1:C:267:MET:HE3	1.74	0.69
1:A:355:PHE:HB2	1:A:383:ARG:NH2	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:VAL:HG13	1:A:463:LEU:HB2	1.74	0.68
1:A:341:ASN:HD21	1:A:343:GLN:NE2	1.91	0.68
1:C:501:GLY:HA3	1:C:506:GLU:OE1	1.93	0.68
1:C:389:GLU:O	1:C:393:THR:HG23	1.94	0.68
1:A:331:ILE:HD11	1:A:478:THR:HG21	1.75	0.67
1:B:355:PHE:HD1	1:B:356:HIS:H	1.43	0.67
1:B:355:PHE:HD1	1:B:356:HIS:N	1.93	0.67
1:B:354:GLY:O	1:B:355:PHE:HB2	1.96	0.66
1:A:311:MET:CE	1:A:413:LEU:HD23	2.26	0.66
1:B:341:ASN:HD21	1:B:378:ARG:HG2	1.61	0.66
1:C:480:LYS:HZ3	1:C:506:GLU:HG2	1.60	0.65
1:D:427:HIS:CD2	1:D:523:HIS:HE1	2.11	0.65
1:A:501:GLY:HA3	1:A:506:GLU:OE1	1.97	0.65
1:A:520:ILE:HD13	1:A:526:LEU:HD23	1.78	0.65
1:C:452:ILE:HB	1:C:453:PRO:HD3	1.77	0.65
1:B:427:HIS:CD2	1:B:523:HIS:HE1	2.07	0.65
1:B:537:TYR:O	1:C:269:ARG:NH2	2.28	0.64
1:A:520:ILE:HD13	1:A:526:LEU:CD2	2.27	0.64
1:B:345:LEU:HG	1:B:385:ARG:HH21	1.62	0.64
1:B:375:ASP:N	1:B:378:ARG:HD2	2.13	0.64
1:C:315:LEU:O	1:C:315:LEU:HD23	1.98	0.63
1:B:452:ILE:HB	1:B:453:PRO:HD3	1.80	0.63
1:D:501:GLY:HA3	1:D:506:GLU:OE1	2.00	0.62
1:A:321:PHE:CE1	1:A:386:ARG:HG2	2.35	0.62
1:C:444:VAL:HG11	1:C:487:ILE:HD13	1.82	0.62
1:B:444:VAL:HG11	1:B:487:ILE:HD13	1.82	0.62
1:A:481:GLU:HG3	1:A:513:HIS:CE1	2.32	0.61
1:C:385:ARG:O	1:C:389:GLU:HG3	2.00	0.61
1:D:374:VAL:O	1:D:378:ARG:HD3	2.01	0.60
1:A:311:MET:HE2	1:A:413:LEU:HD23	1.84	0.60
1:A:321:PHE:HE1	1:A:386:ARG:HG2	1.67	0.60
1:B:340:ASP:OD1	1:B:341:ASN:N	2.31	0.60
1:D:458:VAL:HG13	1:D:463:LEU:HB2	1.83	0.60
1:B:389:GLU:O	1:B:393:THR:HG23	2.01	0.59
1:C:304:ILE:HG21	1:C:417:LEU:HD12	1.84	0.59
1:B:339:ASP:CB	1:B:377:MET:HB3	2.31	0.59
1:B:480:LYS:HD2	1:B:505:GLU:HG2	1.85	0.58
1:B:481:GLU:OE2	1:B:512:LYS:HD2	2.03	0.58
1:B:312:ILE:HD13	1:B:457:LYS:HG2	1.84	0.58
1:C:284:SER:HB3	1:C:290:PHE:HB2	1.86	0.58
1:B:496:VAL:HG11	1:C:267:MET:CE	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:LEU:C	1:C:315:LEU:HD23	2.24	0.58
1:B:375:ASP:CG	1:B:376:TRP:H	2.07	0.58
1:A:484:PHE:CD1	1:A:515:MET:HE3	2.38	0.57
1:A:333:VAL:HG22	4:A:58:HOH:O	2.05	0.57
1:A:452:ILE:HB	1:A:453:PRO:HD3	1.87	0.57
1:C:450:GLN:O	1:C:453:PRO:HD2	2.04	0.56
1:B:350:PHE:HB3	1:B:383:ARG:NH1	2.18	0.56
1:B:315:LEU:CD1	1:B:402:ILE:HD11	2.36	0.56
1:C:350:PHE:HD2	1:C:383:ARG:NH1	2.04	0.56
1:C:402:ILE:HG23	1:C:406:LYS:CB	2.36	0.56
1:A:331:ILE:HD11	1:A:478:THR:CG2	2.34	0.56
1:C:290:PHE:CE2	1:C:421:THR:HA	2.40	0.56
1:B:336:VAL:HG12	1:B:336:VAL:O	2.06	0.56
1:A:530:ARG:HB3	1:A:530:ARG:NH1	2.21	0.55
1:D:339:ASP:OD2	1:D:339:ASP:N	2.38	0.55
1:B:345:LEU:HB2	1:B:348:TYR:HB2	1.88	0.55
1:B:329:ASP:CG	1:B:477:LYS:HE3	2.26	0.55
1:A:319:HIS:HE1	4:A:30:HOH:O	1.89	0.55
1:A:530:ARG:NH2	1:A:534:GLU:OE1	2.40	0.55
1:A:385:ARG:O	1:A:389:GLU:HG3	2.06	0.55
1:A:497:TYR:O	1:A:516:PRO:HG2	2.07	0.55
1:B:355:PHE:HD2	1:B:383:ARG:HE	1.55	0.54
1:D:353:ASP:OD1	1:D:355:PHE:HB2	2.07	0.54
1:D:339:ASP:OD1	1:D:377:MET:HB3	2.08	0.54
1:D:507:GLU:HG3	1:D:511:LYS:HE3	1.88	0.54
1:B:485:GLU:O	1:B:489:GLN:HG2	2.07	0.54
1:B:345:LEU:HB2	1:B:348:TYR:CB	2.37	0.54
1:D:510:ALA:HA	1:D:515:MET:CE	2.37	0.54
1:B:329:ASP:HB2	1:B:477:LYS:HD2	1.89	0.54
1:D:375:ASP:O	1:D:379:LYS:HG3	2.08	0.54
1:C:339:ASP:O	1:C:378:ARG:HA	2.08	0.54
1:C:322:PHE:CZ	1:C:326:GLU:HG3	2.42	0.54
1:D:308:MET:HE3	1:D:312:ILE:HG13	1.90	0.54
1:A:290:PHE:CE2	1:A:421:THR:HA	2.43	0.54
1:A:325:LEU:HD22	1:A:384:TYR:CE1	2.42	0.53
1:B:339:ASP:HA	1:B:378:ARG:NH2	2.23	0.53
1:C:383:ARG:HG2	1:C:383:ARG:NH1	2.17	0.53
1:D:339:ASP:O	1:D:378:ARG:HA	2.08	0.53
1:B:494:LYS:HG2	1:B:494:LYS:O	2.07	0.53
1:B:353:ASP:HB2	1:B:379:LYS:NZ	2.23	0.53
1:D:345:LEU:HG	1:D:385:ARG:NH2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:THR:OG1	1:C:289:THR:HG23	2.09	0.53
1:C:308:MET:HA	1:C:308:MET:HE3	1.91	0.53
1:B:385:ARG:O	1:B:389:GLU:HG3	2.09	0.53
1:A:386:ARG:O	1:A:390:MET:HG2	2.08	0.53
1:D:510:ALA:HA	1:D:515:MET:HE2	1.92	0.52
1:A:481:GLU:OE2	1:A:512:LYS:HD3	2.09	0.52
1:B:355:PHE:CD1	1:B:356:HIS:N	2.75	0.52
1:B:332:HIS:ND1	1:B:333:VAL:N	2.57	0.52
1:C:355:PHE:HB3	1:C:383:ARG:HH21	1.74	0.52
1:A:485:GLU:O	1:A:489:GLN:HG2	2.09	0.52
1:A:303:ARG:HG2	1:A:307:MET:HE3	1.91	0.52
1:B:330:GLN:HA	1:B:330:GLN:NE2	2.25	0.52
1:B:386:ARG:HG2	1:B:386:ARG:HH11	1.75	0.52
1:D:468:PRO:HG2	1:D:471:ASN:HB2	1.92	0.52
1:A:378:ARG:HH11	1:A:378:ARG:HB3	1.74	0.51
1:C:496:VAL:HG23	1:C:496:VAL:O	2.10	0.51
1:B:345:LEU:CB	1:B:348:TYR:HB2	2.40	0.51
1:A:378:ARG:HH11	1:A:378:ARG:CB	2.24	0.51
1:C:268:GLU:O	1:C:496:VAL:HG22	2.09	0.51
1:C:308:MET:HE3	1:C:311:MET:HB2	1.92	0.51
1:C:375:ASP:HA	1:C:378:ARG:HH12	1.74	0.51
1:D:312:ILE:HD13	1:D:457:LYS:HG2	1.92	0.51
1:D:310:GLU:O	1:D:314:ASN:HB2	2.10	0.51
1:D:293:ARG:NH2	1:D:521:SER:O	2.42	0.50
1:C:386:ARG:O	1:C:390:MET:HG2	2.11	0.50
1:B:442:VAL:HG22	1:B:443:ASN:N	2.26	0.50
1:D:331:ILE:HG13	1:D:477:LYS:HD3	1.93	0.50
1:C:458:VAL:HG13	1:C:463:LEU:HB2	1.93	0.50
1:B:355:PHE:HD2	1:B:383:ARG:NE	2.09	0.50
1:B:329:ASP:HB2	1:B:477:LYS:CD	2.42	0.49
1:D:520:ILE:HD11	1:D:529:LEU:CD2	2.42	0.49
1:D:452:ILE:HB	1:D:453:PRO:HD3	1.94	0.49
1:C:448:THR:HG23	1:C:480:LYS:HE3	1.94	0.49
1:C:468:PRO:HG2	1:C:471:ASN:OD1	2.12	0.49
1:C:355:PHE:CB	1:C:383:ARG:HH21	2.25	0.49
1:B:326:GLU:HG3	1:B:326:GLU:O	2.12	0.49
1:B:293:ARG:NH2	1:B:521:SER:O	2.40	0.49
1:A:269:ARG:NH1	1:A:536:GLU:OE2	2.46	0.49
1:D:327:ASP:O	1:D:328:CYS:C	2.51	0.49
1:B:317:ASP:OD1	1:B:322:PHE:HB3	2.13	0.49
1:C:484:PHE:HB3	1:C:515:MET:CE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:LEU:HG	1:B:385:ARG:NH2	2.27	0.48
1:C:484:PHE:CD1	1:C:515:MET:HE1	2.48	0.48
1:A:538:LEU:CD2	1:D:516:PRO:HB3	2.43	0.48
1:A:315:LEU:HD23	1:A:315:LEU:O	2.14	0.48
1:B:340:ASP:CG	1:B:341:ASN:H	2.17	0.48
1:D:481:GLU:OE1	1:D:512:LYS:HD2	2.13	0.48
1:B:401:LEU:HG	1:B:402:ILE:HD12	1.94	0.48
1:D:468:PRO:HG2	1:D:471:ASN:CG	2.34	0.48
1:D:418:GLU:OE2	1:D:425:LEU:HB3	2.13	0.48
1:B:344:ASP:C	1:B:346:SER:H	2.18	0.47
1:C:497:TYR:O	1:C:516:PRO:HG2	2.14	0.47
1:B:451:LEU:O	1:B:455:LEU:HG	2.13	0.47
1:C:339:ASP:N	1:C:339:ASP:OD1	2.48	0.47
1:A:311:MET:HE1	1:A:413:LEU:HD23	1.95	0.47
1:C:336:VAL:O	1:C:381:ALA:HB2	2.14	0.47
1:D:303:ARG:HH22	1:D:416:GLU:CD	2.17	0.47
1:D:315:LEU:O	1:D:315:LEU:HD23	2.15	0.47
1:B:507:GLU:CG	1:B:511:LYS:HE2	2.45	0.46
1:B:375:ASP:CG	1:B:376:TRP:N	2.69	0.46
1:B:308:MET:CE	1:B:460:LEU:HD13	2.45	0.46
1:B:336:VAL:HG11	1:B:380:LEU:CD1	2.44	0.46
1:C:480:LYS:HG3	1:C:505:GLU:OE2	2.16	0.46
1:B:480:LYS:HB2	1:B:505:GLU:HG2	1.97	0.46
1:B:355:PHE:CD2	1:B:383:ARG:NE	2.83	0.46
1:D:268:GLU:HA	1:D:440:ASN:O	2.15	0.46
1:C:383:ARG:CG	1:C:383:ARG:NH1	2.79	0.46
1:B:501:GLY:HA3	1:B:506:GLU:OE1	2.15	0.46
1:D:535:LEU:O	1:D:536:GLU:HB2	2.16	0.46
1:D:321:PHE:CG	1:D:383:ARG:HD2	2.50	0.46
1:D:330:GLN:OE1	1:D:336:VAL:HG13	2.16	0.46
1:B:510:ALA:HA	1:B:515:MET:CE	2.46	0.46
1:D:316:ALA:HB1	1:D:322:PHE:HB2	1.97	0.46
1:B:345:LEU:C	1:B:347:THR:N	2.70	0.45
1:A:427:HIS:HD2	1:A:523:HIS:HD2	1.64	0.45
1:A:418:GLU:OE2	1:A:425:LEU:HB3	2.16	0.45
1:C:304:ILE:CG2	1:C:417:LEU:HD12	2.45	0.45
1:D:480:LYS:HB2	1:D:505:GLU:HG2	1.99	0.45
1:B:380:LEU:C	1:B:380:LEU:HD13	2.37	0.45
1:B:450:GLN:O	1:B:453:PRO:HD2	2.17	0.45
1:C:386:ARG:HH11	1:C:386:ARG:HG2	1.82	0.45
1:C:320:LEU:HD22	1:C:387:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:PHE:HZ	1:B:380:LEU:HD23	1.82	0.44
1:A:496:VAL:HG23	1:A:496:VAL:O	2.17	0.44
1:C:285:LEU:HD11	1:C:417:LEU:HD11	1.99	0.44
1:C:478:THR:HB	1:C:482:SER:OG	2.17	0.44
1:B:402:ILE:CG2	1:B:406:LYS:HB3	2.48	0.44
1:B:339:ASP:HA	1:B:378:ARG:HH22	1.82	0.44
1:B:458:VAL:HG13	1:B:463:LEU:HB2	1.99	0.44
1:A:356:HIS:CD2	1:A:356:HIS:N	2.85	0.44
1:A:293:ARG:HD2	1:A:294:TYR:CZ	2.53	0.44
1:C:480:LYS:HZ2	1:C:506:GLU:HG2	1.80	0.44
1:B:308:MET:HE1	1:B:460:LEU:HD13	1.99	0.44
1:A:538:LEU:HD22	1:D:516:PRO:HB3	2.00	0.44
1:D:430:LYS:HB3	1:D:530:ARG:HD2	1.99	0.44
1:C:348:TYR:C	1:C:348:TYR:CD2	2.91	0.44
1:B:311:MET:CE	1:B:413:LEU:HD23	2.48	0.44
1:C:506:GLU:H	1:C:506:GLU:HG3	1.43	0.44
1:C:317:ASP:OD1	1:C:322:PHE:HB3	2.18	0.44
1:D:320:LEU:HD22	1:D:387:VAL:HG13	2.00	0.44
1:B:268:GLU:HA	1:B:440:ASN:O	2.18	0.44
1:D:333:VAL:HG11	1:D:469:ILE:HD11	2.00	0.43
1:D:427:HIS:CD2	1:D:523:HIS:CE1	2.92	0.43
1:D:507:GLU:O	1:D:511:LYS:HG3	2.18	0.43
1:B:493:ARG:HG2	1:B:493:ARG:O	2.17	0.43
1:B:308:MET:HE3	1:B:308:MET:O	2.17	0.43
1:B:404:THR:N	1:B:405:PRO:HD2	2.34	0.43
1:B:463:LEU:O	1:B:466:VAL:HG22	2.18	0.43
1:B:468:PRO:HG2	1:B:471:ASN:CG	2.39	0.43
1:B:298:THR:O	1:B:302:VAL:HG23	2.19	0.43
1:C:414:ARG:HD2	4:C:96:HOH:O	2.19	0.43
1:C:355:PHE:CB	1:C:383:ARG:NH2	2.81	0.43
1:C:434:LEU:HD12	1:C:434:LEU:HA	1.84	0.43
1:B:491:PHE:HB2	1:B:497:TYR:OH	2.18	0.43
1:B:484:PHE:O	1:B:488:MET:HG3	2.18	0.43
1:B:329:ASP:HB2	1:B:477:LYS:CE	2.49	0.42
1:D:350:PHE:CD2	1:D:383:ARG:HD3	2.54	0.42
1:A:434:LEU:HA	1:A:434:LEU:HD12	1.87	0.42
1:D:520:ILE:HD11	1:D:529:LEU:HD22	2.01	0.42
1:A:519:ARG:HG2	1:A:520:ILE:N	2.34	0.42
1:B:345:LEU:C	1:B:347:THR:H	2.23	0.42
1:C:404:THR:HG23	1:C:405:PRO:HA	2.01	0.42
1:A:484:PHE:HB3	1:A:515:MET:CE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:ILE:HD11	1:B:478:THR:HG21	2.01	0.42
1:B:444:VAL:HG11	1:B:487:ILE:CD1	2.48	0.42
1:B:315:LEU:HD12	1:B:402:ILE:HD11	2.02	0.42
1:D:308:MET:O	1:D:312:ILE:HG13	2.20	0.42
1:B:339:ASP:HB3	1:B:377:MET:CB	2.45	0.41
1:C:404:THR:CG2	1:C:405:PRO:HA	2.50	0.41
1:A:343:GLN:O	1:A:385:ARG:NH2	2.45	0.41
1:A:484:PHE:HB3	1:A:515:MET:HE1	2.02	0.41
1:A:267:MET:CE	1:D:496:VAL:HG11	2.46	0.41
1:C:483:CYS:O	1:C:487:ILE:HG13	2.19	0.41
1:C:289:THR:HG22	1:D:426:THR:OG1	2.21	0.41
1:A:269:ARG:NH1	1:A:536:GLU:OE1	2.53	0.41
1:A:355:PHE:CZ	1:A:380:LEU:HD23	2.54	0.41
1:C:325:LEU:HD13	1:C:384:TYR:CZ	2.56	0.41
1:B:480:LYS:HZ3	1:B:506:GLU:HG2	1.86	0.41
1:D:510:ALA:HA	1:D:515:MET:HE3	2.03	0.41
1:A:504:VAL:HG23	1:A:505:GLU:N	2.35	0.41
1:A:536:GLU:HA	1:D:517:PHE:O	2.21	0.41
1:A:407:ARG:NH1	1:A:408:GLU:OE1	2.48	0.41
1:B:341:ASN:HD21	1:B:378:ARG:CG	2.31	0.41
1:B:386:ARG:O	1:B:390:MET:HG3	2.21	0.41
1:B:507:GLU:HG3	1:B:511:LYS:HE2	2.02	0.41
1:A:480:LYS:HG3	1:A:505:GLU:OE2	2.21	0.41
1:B:527:GLU:HA	1:B:527:GLU:OE1	2.20	0.41
1:D:468:PRO:HG2	1:D:471:ASN:CB	2.51	0.41
1:B:391:TYR:O	1:B:395:LYS:HB3	2.20	0.41
1:C:280:ILE:HD11	1:C:457:LYS:HD3	2.02	0.41
1:B:418:GLU:OE1	1:B:423:LEU:HA	2.21	0.40
1:A:312:ILE:HD13	1:A:457:LYS:HG2	2.03	0.40
1:A:520:ILE:CD1	1:A:526:LEU:HD23	2.48	0.40
1:A:349:ASN:ND2	1:A:352:ALA:CB	2.80	0.40
1:B:308:MET:O	1:B:312:ILE:HG13	2.21	0.40
1:D:514:ASN:N	1:D:514:ASN:HD22	2.18	0.40
1:A:293:ARG:NH1	4:A:47:HOH:O	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	255/274 (93%)	243 (95%)	11 (4%)	1 (0%)	39	61
1	B	249/274 (91%)	233 (94%)	11 (4%)	5 (2%)	9	15
1	C	255/274 (93%)	234 (92%)	18 (7%)	3 (1%)	16	29
1	D	252/274 (92%)	233 (92%)	15 (6%)	4 (2%)	12	21
All	All	1011/1096 (92%)	943 (93%)	55 (5%)	13 (1%)	15	26

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	329	ASP
1	B	342	GLY
1	B	345	LEU
1	D	328	CYS
1	D	477	LYS
1	B	341	ASN
1	B	355	PHE
1	D	336	VAL
1	C	403	GLY
1	D	326	GLU
1	C	354	GLY
1	C	469	ILE
1	A	373	GLY

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	227/237 (96%)	217 (96%)	10 (4%)	35 60
1	B	223/237 (94%)	212 (95%)	11 (5%)	31 55
1	C	227/237 (96%)	214 (94%)	13 (6%)	25 46
1	D	224/237 (94%)	215 (96%)	9 (4%)	38 64
All	All	901/948 (95%)	858 (95%)	43 (5%)	31 55

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	353	ASP
1	A	378	ARG
1	A	380	LEU
1	A	386	ARG
1	A	393	THR
1	A	417	LEU
1	A	490	ARG
1	A	493	ARG
1	A	506	GLU
1	A	530	ARG
1	B	268	GLU
1	B	339	ASP
1	B	341	ASN
1	B	345	LEU
1	B	355	PHE
1	B	378	ARG
1	B	412	GLN
1	B	414	ARG
1	B	506	GLU
1	B	526	LEU
1	B	530	ARG
1	C	329	ASP
1	C	339	ASP
1	C	344	ASP
1	C	348	TYR
1	C	353	ASP
1	C	356	HIS
1	C	375	ASP
1	C	382	PHE
1	C	402	ILE
1	C	414	ARG
1	C	417	LEU
1	C	466	VAL

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Mol	Chain	Res	Type
1	C	514	ASN
1	D	296	LYS
1	D	308	MET
1	D	330	GLN
1	D	339	ASP
1	D	378	ARG
1	D	386	ARG
1	D	414	ARG
1	D	476	THR
1	D	526	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	283	HIS
1	A	319	HIS
1	A	343	GLN
1	A	349	ASN
1	A	397	ASN
1	A	412	GLN
1	A	427	HIS
1	A	436	ASN
1	A	508	GLN
1	A	513	HIS
1	B	283	HIS
1	B	319	HIS
1	B	330	GLN
1	B	341	ASN
1	B	412	GLN
1	B	427	HIS
1	B	523	HIS
1	C	283	HIS
1	C	319	HIS
1	C	412	GLN
1	D	397	ASN
1	D	427	HIS
1	D	489	GLN
1	D	513	HIS
1	D	514	ASN
1	D	523	HIS

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	BEF	A	801	1	0,3,3	0.00	-	0,3,3	0.00	-
2	BEF	B	802	1	0,3,3	0.00	-	0,3,3	0.00	-
2	BEF	C	803	1	0,3,3	0.00	-	0,3,3	0.00	-
2	BEF	D	804	1	0,3,3	0.00	-	0,3,3	0.00	-

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	BEF	A	801	1	-	0/0/0/0	0/0/0/0
2	BEF	B	802	1	-	0/0/0/0	0/0/0/0
2	BEF	C	803	1	-	0/0/0/0	0/0/0/0
2	BEF	D	804	1	-	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.

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	259/274 (94%)	0.07	6 (2%) 64 67	26, 37, 61, 78	0
1	B	253/274 (92%)	0.57	32 (12%) 5 5	28, 48, 80, 80	0
1	C	259/274 (94%)	0.53	33 (12%) 5 5	31, 48, 80, 80	0
1	D	256/274 (93%)	0.35	19 (7%) 17 19	28, 44, 80, 80	0
All	All	1027/1096 (93%)	0.38	90 (8%) 12 13	26, 44, 80, 80	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	355	PHE	9.0
1	B	356	HIS	6.8
1	D	345	LEU	5.9
1	C	345	LEU	5.8
1	C	374	VAL	5.6
1	B	382	PHE	5.6
1	C	338	SER	5.4
1	B	352	ALA	5.4
1	C	337	SER	5.2
1	C	346	SER	5.1
1	B	354	GLY	5.1
1	B	329	ASP	5.0
1	C	382	PHE	4.8
1	B	378	ARG	4.7
1	B	337	SER	4.6
1	C	344	ASP	4.6
1	B	379	LYS	4.5
1	C	355	PHE	4.5
1	C	380	LEU	4.4
1	C	352	ALA	4.3
1	D	356	HIS	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	342	GLY	4.1
1	C	347	THR	4.0
1	B	376	TRP	4.0
1	C	377	MET	4.0
1	B	380	LEU	3.9
1	C	376	TRP	3.9
1	B	344	ASP	3.9
1	C	375	ASP	3.9
1	C	342	GLY	3.8
1	B	347	THR	3.8
1	C	378	ARG	3.8
1	D	343	GLN	3.7
1	C	350	PHE	3.6
1	B	493	ARG	3.6
1	C	379	LYS	3.5
1	C	348	TYR	3.5
1	B	338	SER	3.3
1	B	350	PHE	3.3
1	B	383	ARG	3.2
1	C	373	GLY	3.2
1	D	355	PHE	3.2
1	D	350	PHE	3.2
1	D	351	SER	3.2
1	B	343	GLN	3.1
1	C	340	ASP	3.1
1	B	377	MET	3.1
1	B	494	LYS	3.1
1	B	345	LEU	3.1
1	B	340	ASP	3.1
1	B	341	ASN	3.0
1	B	353	ASP	3.0
1	D	378	ARG	3.0
1	A	265	SER	2.9
1	C	336	VAL	2.9
1	B	339	ASP	2.9
1	C	339	ASP	2.9
1	A	355	PHE	2.9
1	D	372	GLY	2.9
1	D	382	PHE	2.9
1	B	348	TYR	2.8
1	C	343	GLN	2.8
1	D	352	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	356	HIS	2.7
1	A	356	HIS	2.7
1	D	337	SER	2.7
1	D	347	THR	2.7
1	B	489	GLN	2.6
1	B	351	SER	2.6
1	C	265	SER	2.6
1	D	376	TRP	2.6
1	C	327	ASP	2.5
1	C	325	LEU	2.4
1	D	348	TYR	2.4
1	B	384	TYR	2.4
1	D	338	SER	2.4
1	C	493	ARG	2.4
1	A	373	GLY	2.3
1	A	376	TRP	2.3
1	C	372	GLY	2.3
1	B	328	CYS	2.3
1	C	353	ASP	2.3
1	C	328	CYS	2.3
1	C	384	TYR	2.2
1	D	375	ASP	2.2
1	D	383	ARG	2.2
1	B	375	ASP	2.1
1	A	494	LYS	2.1
1	D	344	ASP	2.1
1	D	346	SER	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
3	MG	B	702	1/1	0.90	0.20	3.41	44,44,44,44	0
3	MG	D	704	1/1	0.90	0.20	2.61	43,43,43,43	0
3	MG	A	701	1/1	0.81	0.19	0.97	36,36,36,36	0
2	BEF	D	804	4/4	0.96	0.16	-0.15	35,36,37,39	0
3	MG	C	703	1/1	0.90	0.16	-0.28	39,39,39,39	0
2	BEF	A	801	4/4	0.97	0.12	-1.38	33,33,34,36	0
2	BEF	B	802	4/4	0.94	0.09	-2.46	43,43,44,44	0
2	BEF	C	803	4/4	0.96	0.10	-3.75	40,40,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.