Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2023 – 11:27 AM EDT

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

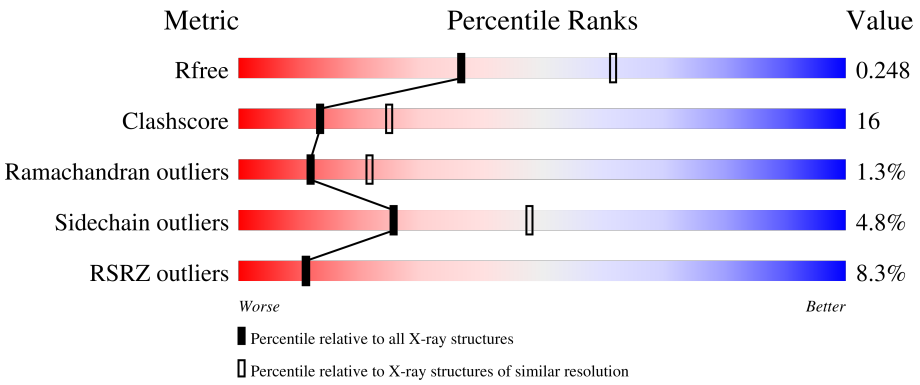
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 of 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 <=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	5%, 65%, 26%, • 7%

2 Entry composition (i)

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.

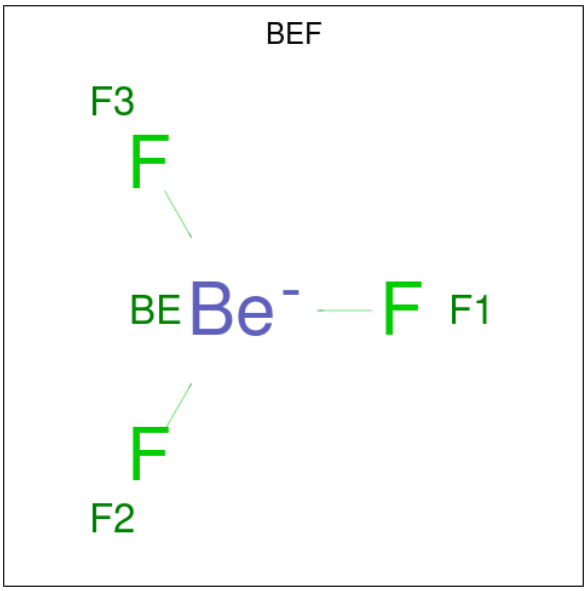
- Molecule 1 is a protein called Eyes absent homolog 2 (Drosophila).

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

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
			Total	Be	F		
2	A	1	4	1	3	0	0
2	B	1	4	1	3	0	0
2	C	1	4	1	3	0	0
2	D	1	4	1	3	0	0

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

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

- Molecule 4 is water.

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

Continued on next page...

Continued from previous page...

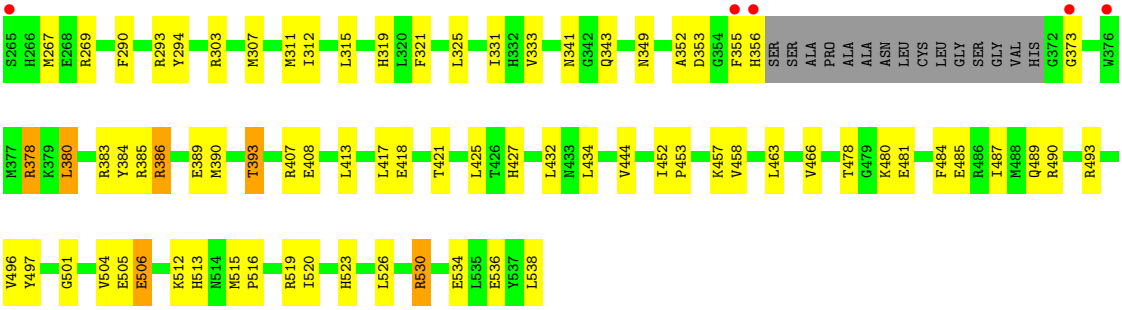
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	32	32	32	0	0
			Total	O		
4	C	22	22	22	0	0
			Total	O		
4	D	35	35	35	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Eyes absent homolog 2 (Drosophila)

Chain A:

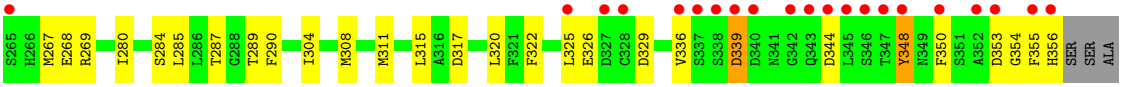


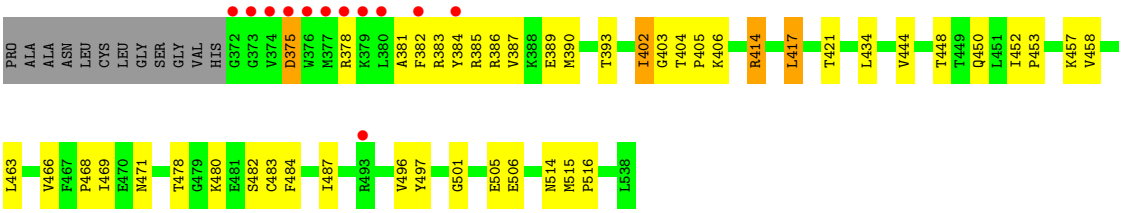
• Molecule 1: Eyes absent homolog 2 (Drosophila)

Chain B:

• Molecule 1: Eyes absent homolog 2 (Drosophila)

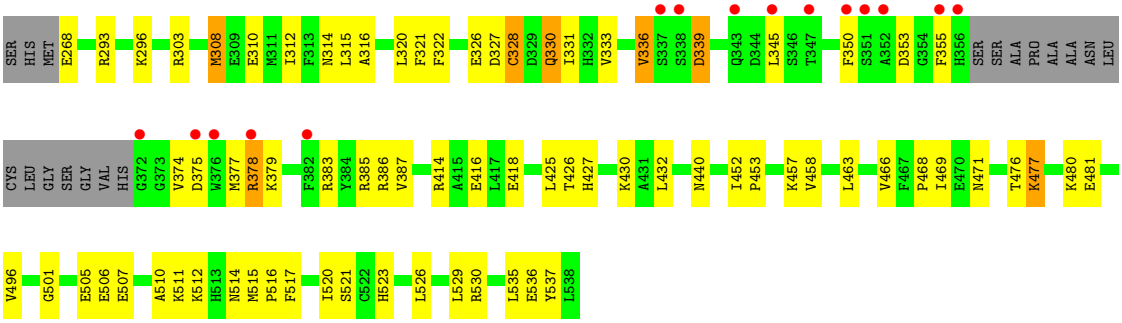
Chain C:





- Molecule 1: Eyes absent homolog 2 (Drosophila)

Chain D:



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	Depositor
R, R_{free}	0.224 , 0.254 0.216 , 0.248	Depositor DCC
R_{free} test set	3441 reflections (5.09%)	wwPDB-VP
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
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -k,-h,-l	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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 (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	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

Continued on next page...

Continued from previous page...

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:C:383:ARG:HG2	1:C:383:ARG:HH11	1.44	0.82
1:D:427:HIS:HD2	1:D:523:HIS:HE1	1.25	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:A:432:LEU:HB3	1:A:466:VAL:HG21	1.69	0.74
1:B:350:PHE:HB3	1:B:383:ARG:HH12	1.53	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:HH11	1:A:530:ARG:HB3	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

Continued on next page...

Continued from previous page...

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:389:GLU:O	1:C:393:THR:HG23	1.94	0.68
1:C:501:GLY:HA3	1:C:506:GLU:OE1	1.93	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:A:501:GLY:HA3	1:A:506:GLU:OE1	1.97	0.65
1:D:427:HIS:CD2	1:D:523:HIS:HE1	2.11	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:HD23	1:C:315:LEU:O	1.98	0.63
1:B:452:ILE:HB	1:B:453:PRO:HD3	1.80	0.63
1:A:321:PHE:CE1	1:A:386:ARG:HG2	2.35	0.62
1:D:501:GLY:HA3	1:D:506:GLU:OE1	2.00	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:LEU:HD23	1:C:315:LEU:C	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: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: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: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:329:ASP:CG	1:B:477:LYS:HE3	2.26	0.55
1:B:345:LEU:HB2	1:B:348:TYR:HB2	1.88	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:B:485:GLU:O	1:B:489:GLN:HG2	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: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:322:PHE:CZ	1:C:326:GLU:HG3	2.42	0.54
1:C:339:ASP:O	1:C:378:ARG:HA	2.08	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:O	1:B:494:LYS:HG2	2.07	0.53
1:B:353:ASP:HB2	1:B:379:LYS:NZ	2.23	0.53
1:C:287:THR:OG1	1:C:289:THR:HG23	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:LEU:HG	1:D:385:ARG:NH2	2.23	0.53
1:C:308:MET:HA	1:C:308:MET:HE3	1.91	0.53
1:A:386:ARG:O	1:A:390:MET:HG2	2.08	0.53
1:B:385:ARG:O	1:B:389:GLU:HG3	2.09	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:332:HIS:ND1	1:B:333:VAL:N	2.57	0.52
1:B:355:PHE:CD1	1:B:356:HIS:N	2.75	0.52
1:C:355:PHE:HB3	1:C:383:ARG:HH21	1.74	0.52
1:A:303:ARG:HG2	1:A:307:MET:HE3	1.91	0.52
1:A:485:GLU:O	1:A:489:GLN:HG2	2.09	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:310:GLU:O	1:D:314:ASN:HB2	2.10	0.51
1:D:312:ILE:HD13	1:D:457:LYS:HG2	1.92	0.51
1:B:442:VAL:HG22	1:B:443:ASN:N	2.26	0.50
1:C:386:ARG:O	1:C:390:MET:HG2	2.11	0.50
1:D:293:ARG:NH2	1:D:521:SER:O	2.42	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:452:ILE:HB	1:D:453:PRO:HD3	1.94	0.49
1:D:520:ILE:HD11	1:D:529:LEU:CD2	2.42	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:B:326:GLU:O	1:B:326:GLU:HG3	2.12	0.49
1:C:355:PHE:CB	1:C:383:ARG:HH21	2.25	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:LEU:CD2	1:D:516:PRO:HB3	2.43	0.48
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:315:LEU:O	1:A:315:LEU:HD23	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:418:GLU:OE2	1:D:425:LEU:HB3	2.13	0.48
1:D:468:PRO:HG2	1:D:471:ASN:CG	2.34	0.48
1:B:344:ASP:C	1:B:346:SER:H	2.18	0.47
1:B:451:LEU:O	1:B:455:LEU:HG	2.13	0.47
1:C:497:TYR:O	1:C:516:PRO:HG2	2.14	0.47
1:C:339:ASP:OD1	1:C:339:ASP:N	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:308:MET:CE	1:B:460:LEU:HD13	2.45	0.46
1:B:375:ASP:CG	1:B:376:TRP:N	2.69	0.46
1:B:336:VAL:HG11	1:B:380:LEU:CD1	2.44	0.46
1:B:480:LYS:HB2	1:B:505:GLU:HG2	1.97	0.46
1:C:480:LYS:HG3	1:C:505:GLU:OE2	2.16	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:B:501:GLY:HA3	1:B:506:GLU:OE1	2.15	0.46
1:C:383:ARG:NH1	1:C:383:ARG:CG	2.79	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:D:535:LEU:O	1:D:536:GLU:HB2	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:HG2	1:C:386:ARG:HH11	1.82	0.45
1:C:320:LEU:HD22	1:C:387:VAL:HG13	1.99	0.45

Continued on next page...

Continued from previous page...

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:A:356:HIS:N	1:A:356:HIS:CD2	2.85	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:293:ARG:HD2	1:A:294:TYR:CZ	2.53	0.44
1:A:538:LEU:HD22	1:D:516:PRO:HB3	2.00	0.44
1:B:308:MET:HE1	1:B:460:LEU:HD13	1.99	0.44
1:B:311:MET:CE	1:B:413:LEU:HD23	2.48	0.44
1:C:348:TYR:C	1:C:348:TYR:CD2	2.91	0.44
1:C:480:LYS:HZ2	1:C:506:GLU:HG2	1.80	0.44
1:D:430:LYS:HB3	1:D:530:ARG:HD2	1.99	0.44
1:B:268:GLU:HA	1:B:440:ASN:O	2.18	0.44
1:C:317:ASP:OD1	1:C:322:PHE:HB3	2.18	0.44
1:C:506:GLU:H	1:C:506:GLU:HG3	1.43	0.44
1:D:320:LEU:HD22	1:D:387:VAL:HG13	2.00	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:B:493:ARG:O	1:B:493:ARG:HG2	2.17	0.43
1:D:507:GLU:O	1:D:511:LYS:HG3	2.18	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:298:THR:O	1:B:302:VAL:HG23	2.19	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:C:414:ARG:HD2	4:C:96:HOH:O	2.19	0.43
1:B:491:PHE:HB2	1:B:497:TYR:OH	2.18	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: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:A:434:LEU:HD12	1:A:434:LEU:HA	1.87	0.42
1:D:350:PHE:CD2	1:D:383:ARG:HD3	2.54	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

Continued on next page...

Continued from previous page...

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:315:LEU:HD12	1:B:402:ILE:HD11	2.02	0.42
1:B:444:VAL:HG11	1:B:487:ILE:CD1	2.48	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:289:THR:HG22	1:D:426:THR:OG1	2.21	0.41
1:C:483:CYS:O	1:C:487:ILE:HG13	2.19	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:A:504:VAL:HG23	1:A:505:GLU:N	2.35	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:407:ARG:NH1	1:A:408:GLU:OE1	2.48	0.41
1:A:536:GLU:HA	1:D:517:PHE:O	2.21	0.41
1:A:480:LYS:HG3	1:A:505:GLU:OE2	2.21	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:B:527:GLU:HA	1:B:527:GLU:OE1	2.20	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:D:468:PRO:HG2	1:D:471:ASN:CB	2.51	0.41
1:A:312:ILE:HD13	1:A:457:LYS:HG2	2.03	0.40
1:B:418:GLU:OE1	1:B:423:LEU:HA	2.21	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 (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	255/274 (93%)	243 (95%)	11 (4%)	1 (0%)	34 54
1	B	249/274 (91%)	233 (94%)	11 (4%)	5 (2%)	7 12
1	C	255/274 (93%)	234 (92%)	18 (7%)	3 (1%)	13 24
1	D	252/274 (92%)	233 (92%)	15 (6%)	4 (2%)	9 17
All	All	1011/1096 (92%)	943 (93%)	55 (5%)	13 (1%)	12 21

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 (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	227/237 (96%)	217 (96%)	10 (4%)	28	52
1	B	223/237 (94%)	212 (95%)	11 (5%)	25	47
1	C	227/237 (96%)	214 (94%)	13 (6%)	20	39
1	D	224/237 (94%)	215 (96%)	9 (4%)	31	56
All	All	901/948 (95%)	858 (95%)	43 (5%)	25	48

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

Continued on next page...

Continued from previous page...

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

Sometimes 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 (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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	D	804	1	0,3,3	-	-	-		
2	BEF	C	803	1	0,3,3	-	-	-		
2	BEF	B	802	1	0,3,3	-	-	-		
2	BEF	A	801	1	0,3,3	-	-	-		

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 (i)

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	259/274 (94%)	-0.02	5 (1%)	66	69	26, 37, 61, 78	0
1	B	253/274 (92%)	0.45	32 (12%)	3	3	28, 48, 80, 80	0
1	C	259/274 (94%)	0.43	33 (12%)	3	3	31, 48, 80, 80	0
1	D	256/274 (93%)	0.23	15 (5%)	22	23	28, 44, 80, 80	0
All	All	1027/1096 (93%)	0.27	85 (8%)	11	11	26, 44, 80, 80	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	355	PHE	8.3
1	B	356	HIS	6.2
1	C	338	SER	5.8
1	C	345	LEU	5.6
1	B	382	PHE	5.5
1	D	345	LEU	5.4
1	C	346	SER	5.2
1	B	352	ALA	5.0
1	C	374	VAL	4.9
1	C	337	SER	4.8
1	B	329	ASP	4.8
1	C	382	PHE	4.8
1	B	378	ARG	4.5
1	C	355	PHE	4.5
1	B	337	SER	4.4
1	D	356	HIS	4.3
1	C	344	ASP	4.3
1	C	380	LEU	4.3
1	B	354	GLY	4.2
1	B	379	LYS	4.2
1	C	352	ALA	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	342	GLY	4.1
1	B	376	TRP	4.0
1	C	376	TRP	4.0
1	C	377	MET	3.9
1	C	347	THR	3.9
1	B	347	THR	3.8
1	B	493	ARG	3.8
1	C	378	ARG	3.7
1	C	342	GLY	3.7
1	B	380	LEU	3.6
1	C	375	ASP	3.6
1	B	344	ASP	3.6
1	C	379	LYS	3.5
1	B	338	SER	3.3
1	D	372	GLY	3.3
1	B	494	LYS	3.3
1	D	343	GLN	3.3
1	C	350	PHE	3.3
1	C	348	TYR	3.2
1	C	373	GLY	3.1
1	B	343	GLN	3.0
1	D	351	SER	3.0
1	B	350	PHE	3.0
1	B	340	ASP	2.9
1	B	377	MET	2.9
1	B	383	ARG	2.9
1	C	343	GLN	2.9
1	D	355	PHE	2.8
1	B	345	LEU	2.8
1	B	339	ASP	2.8
1	B	341	ASN	2.8
1	A	355	PHE	2.8
1	C	340	ASP	2.8
1	A	265	SER	2.7
1	B	353	ASP	2.7
1	C	339	ASP	2.7
1	D	378	ARG	2.7
1	B	489	GLN	2.7
1	D	376	TRP	2.7
1	C	356	HIS	2.6
1	B	348	TYR	2.6
1	C	336	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	350	PHE	2.6
1	A	356	HIS	2.5
1	C	372	GLY	2.5
1	B	351	SER	2.4
1	D	352	ALA	2.4
1	D	347	THR	2.4
1	C	265	SER	2.3
1	B	328	CYS	2.3
1	D	337	SER	2.3
1	B	384	TYR	2.3
1	C	493	ARG	2.2
1	C	328	CYS	2.2
1	A	376	TRP	2.2
1	C	327	ASP	2.2
1	D	375	ASP	2.2
1	D	382	PHE	2.2
1	A	373	GLY	2.2
1	B	375	ASP	2.1
1	C	325	LEU	2.1
1	D	338	SER	2.1
1	C	353	ASP	2.1
1	C	384	TYR	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 monosaccharides 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(Å^2)	Q<0.9
3	MG	A	701	1/1	0.83	0.20	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	B	702	1/1	0.89	0.20	44,44,44,44	0
3	MG	C	703	1/1	0.90	0.17	39,39,39,39	0
3	MG	D	704	1/1	0.91	0.21	43,43,43,43	0
2	BEF	B	802	4/4	0.95	0.09	43,43,44,44	0
2	BEF	C	803	4/4	0.96	0.10	40,40,41,41	0
2	BEF	D	804	4/4	0.96	0.17	35,36,37,39	0
2	BEF	A	801	4/4	0.97	0.13	33,33,34,36	0

6.5 Other polymers (i)

There are no such residues in this entry.