



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:45 AM UTC

PDB ID : 3HB0 / pdb_00003hb0
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

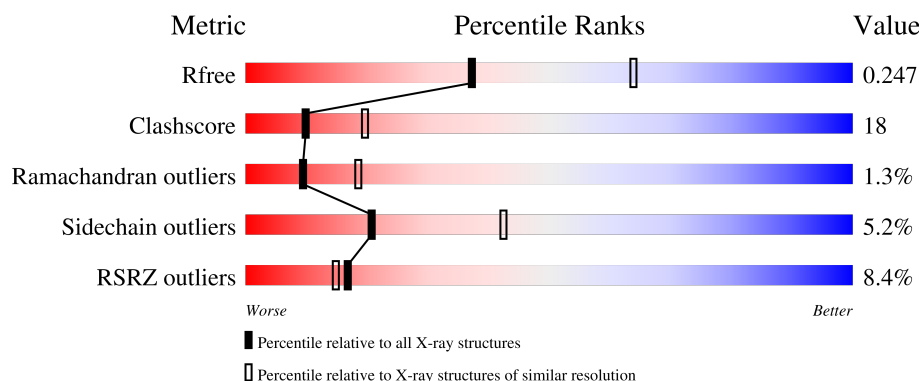
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	274	 3% 63% 30% • 5%
1	B	274	 11% 52% 36% • 8%
1	C	274	 9% 63% 28% • 5%
1	D	274	 8% 61% 28% • 7%

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 (CCD ID: BEF) (formula: BeF₃).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is water.

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

Continued on next page...

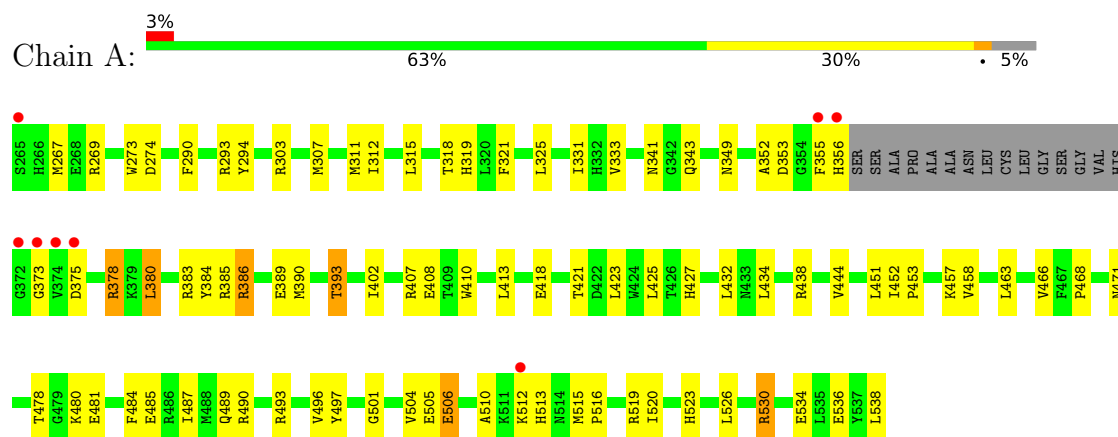
Continued from previous page...

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

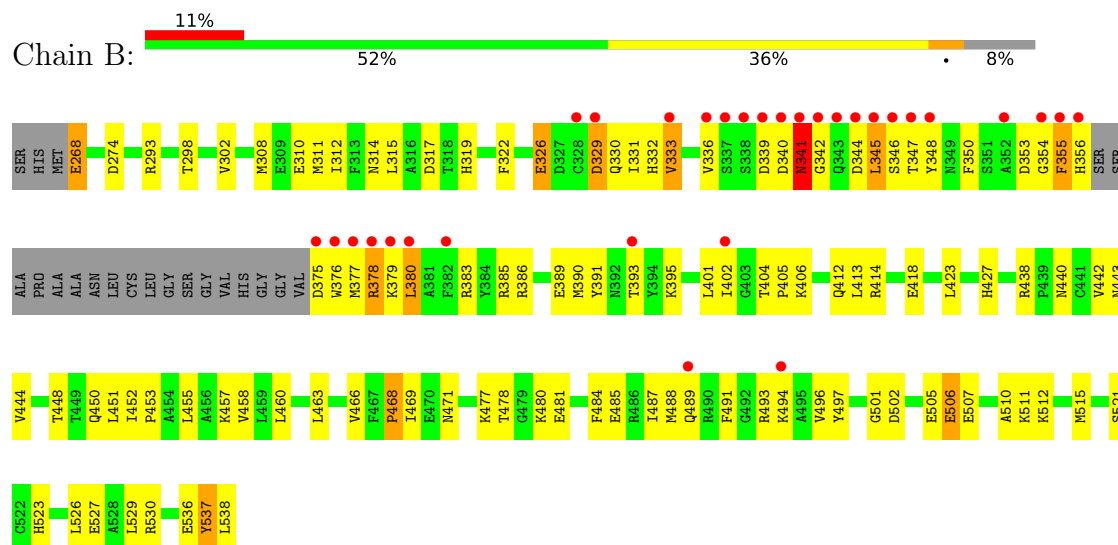
3 Residue-property plots

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.

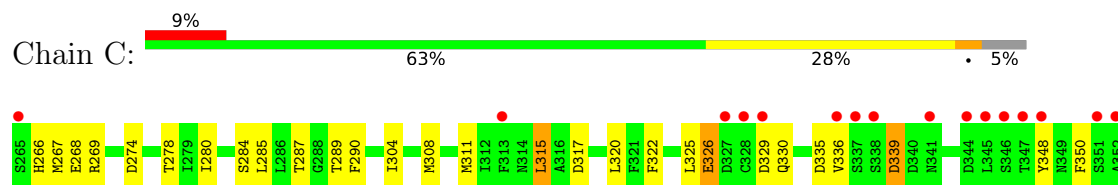
- Molecule 1: Eyes absent homolog 2 (Drosophila)

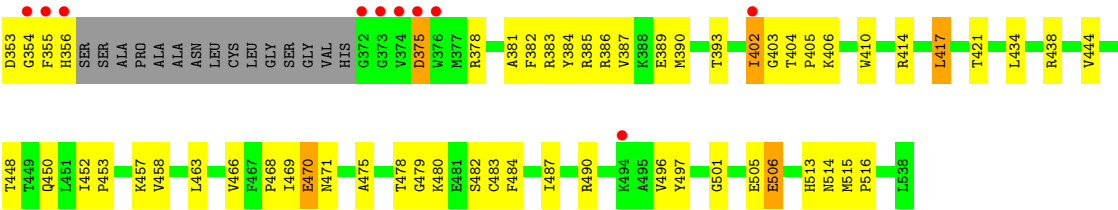


- Molecule 1: Eyes absent homolog 2 (Drosophila)

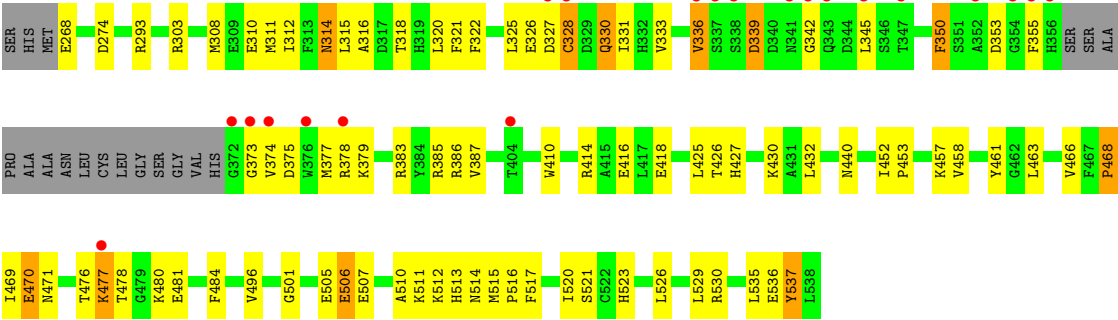


- Molecule 1: Eyes absent homolog 2 (Drosophila)





● Molecule 1: Eyes absent homolog 2 (Drosophila)



4 Data and refinement statistics

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 40.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.3 (40.00-2.50) 93.3 (40.00-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.254 0.217 , 0.247	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)	0.34 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

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: BEF, MG

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	0.46	0/2132	0.94	7/2882 (0.2%)
1	B	0.46	0/2092	0.89	5/2829 (0.2%)
1	C	0.43	0/2132	0.89	7/2882 (0.2%)
1	D	0.46	0/2107	0.92	9/2849 (0.3%)
All	All	0.45	0/8463	0.91	28/11442 (0.2%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	ASP	N-CA-C	-8.00	98.03	110.42
1	B	537	TYR	N-CA-C	-7.54	103.96	113.01
1	C	274	ASP	N-CA-C	-7.10	99.41	110.42
1	A	375	ASP	N-CA-C	-6.69	104.59	112.89
1	C	375	ASP	N-CA-C	-6.58	105.25	113.28
1	B	274	ASP	N-CA-C	-6.43	100.46	110.42
1	C	278	THR	N-CA-C	-6.42	103.51	112.12
1	D	478	THR	N-CA-C	6.40	120.81	113.19
1	C	438	ARG	CA-C-N	6.40	126.15	119.05
1	C	438	ARG	C-N-CA	6.40	126.15	119.05
1	D	342	GLY	N-CA-C	-6.13	106.79	115.43
1	B	468	PRO	N-CA-C	-5.87	101.97	111.19
1	D	274	ASP	N-CA-C	-5.75	102.02	110.52
1	D	468	PRO	N-CA-C	-5.74	102.19	111.19
1	D	537	TYR	N-CA-C	-5.73	105.12	111.71
1	A	438	ARG	CA-C-N	5.65	125.32	119.05
1	A	438	ARG	C-N-CA	5.65	125.32	119.05
1	C	326	GLU	N-CA-C	5.61	117.07	111.07
1	A	318	THR	N-CA-C	5.59	118.31	111.82
1	A	451	LEU	N-CA-C	5.35	117.55	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	318	THR	N-CA-C	5.34	118.01	111.82
1	D	373	GLY	N-CA-C	-5.25	107.27	113.99
1	D	350	PHE	N-CA-C	5.19	117.02	111.36
1	C	335	ASP	N-CA-C	5.18	118.86	112.54
1	D	314	ASN	N-CA-C	-5.14	105.75	112.23
1	A	273	TRP	N-CA-C	5.11	118.04	110.48
1	B	438	ARG	CA-C-N	5.06	124.67	119.05
1	B	438	ARG	C-N-CA	5.06	124.67	119.05

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	68	0
1	B	2049	0	2012	103	0
1	C	2088	0	2048	67	0
1	D	2064	0	2027	59	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
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	288	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 18.

All (288) 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:311:MET:HE2	1:A:413:LEU:HD23	1.39	1.01
1:D:510:ALA:HA	1:D:515:MET:HE3	1.47	0.95
1:B:427:HIS:HD2	1:B:523:HIS:HE1	1.16	0.93
1:C:484:PHE:HB3	1:C:515:MET:HE1	1.55	0.88
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:A:267:MET:HE3	1:D:496:VAL:HG11	1.62	0.82
1:B:310:GLU:O	1:B:314:ASN:HB2	1.80	0.82
1:B:510:ALA:HA	1:B:515:MET:HE3	1.62	0.81
1:A:484:PHE:HB3	1:A:515:MET:HE1	1.63	0.80
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:349:ASN:ND2	1:A:352:ALA:HB3	2.04	0.72
1:A:513:HIS:HB2	1:A:515:MET:HE2	1.71	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:484:PHE:CD1	1:B:515:MET:HE1	2.25	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:B:319:HIS:O	1:B:390:MET:HE1	1.91	0.71
1:A:269:ARG:NH2	1:D:537:TYR:O	2.24	0.70
1:C:513:HIS:HB2	1:C:515:MET:HE2	1.73	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	1.75	0.69
1:D:513:HIS:HB2	1:D:515:MET:HE2	1.74	0.69
1:A:355:PHE:HB2	1:A:383:ARG:NH2	2.08	0.69
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:PHE:HD1	1:B:356:HIS:H	1.43	0.67
1:C:480:LYS:HZ3	1:C:506:GLU:HG2	1.58	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:B:341:ASN:HD21	1:B:378:ARG:HG2	1.61	0.66
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:B:375:ASP:CG	1:B:376:TRP:H	2.07	0.62
1:C:315:LEU:HD23	1:C:315:LEU:C	2.24	0.62
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:C:484:PHE:CB	1:C:515:MET:HE1	2.30	0.61
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:B:311:MET:HE2	1:B:413:LEU:CD2	2.31	0.60
1:D:374:VAL:O	1:D:378:ARG:HD3	2.01	0.60
1:A:321:PHE:HE1	1:A:386:ARG:HG2	1.67	0.60
1:B:329:ASP:CG	1:B:477:LYS:HE3	2.26	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:311:MET:HE2	1:B:413:LEU:HD23	1.84	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:B:484:PHE:HD1	1:B:515:MET:HE1	1.68	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:A:311:MET:HE1	1:A:410:TRP:HD1	1.69	0.58
1:A:333:VAL:HG22	4:A:58:HOH:O	2.05	0.57
1:A:311:MET:HE2	1:A:413:LEU:CD2	2.24	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:B:308:MET:HE1	1:B:460:LEU:HD13	1.88	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: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:A:484:PHE:CB	1:A:515:MET:HE1	2.35	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:C:308:MET:HA	1:C:308:MET:HE3	1.90	0.54
1:B:345:LEU:HB2	1:B:348:TYR:CB	2.37	0.54
1:B:329:ASP:HB2	1:B:477:LYS:HD2	1.89	0.54
1:D:311:MET:HE1	1:D:410:TRP:HB2	1.89	0.54
1:D:327:ASP:O	1:D:328:CYS:C	2.51	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: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

Continued on next page...

Continued from previous page...

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:D:345:LEU:HG	1:D:385:ARG:NH2	2.23	0.53
1:A:386:ARG:O	1:A:390:MET:HG2	2.08	0.53
1:B:340:ASP:CG	1:B:341:ASN:H	2.17	0.53
1:B:385:ARG:O	1:B:389:GLU:HG3	2.09	0.53
1:D:468:PRO:HG2	1:D:471:ASN:CG	2.34	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:485:GLU:O	1:A:489:GLN:HG2	2.09	0.52
1:B:344:ASP:C	1:B:346:SER:H	2.18	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:D:303:ARG:HH22	1:D:416:GLU:CD	2.17	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:B:375:ASP:CG	1:B:376:TRP:N	2.69	0.51
1:C:268:GLU:O	1:C:496:VAL:HG22	2.09	0.51
1:A:303:ARG:HE	1:A:307:MET:HE1	1.75	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:C:308:MET:HE3	1:C:311:MET:HB2	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:C:513:HIS:CB	1:C:515:MET:HE2	2.41	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:B:380:LEU:C	1:B:380:LEU:HD13	2.37	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:308:MET:HE2	1:D:461:TYR:HE1	1.77	0.49
1:B:317:ASP:OD1	1:B:322:PHE:HB3	2.13	0.49
1:A:311:MET:CE	1:A:413:LEU:HD23	2.26	0.48
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:348:TYR:C	1:C:348:TYR:CD2	2.91	0.48
1:A:315:LEU:O	1:A:315:LEU:HD23	2.14	0.48
1:B:345:LEU:C	1:B:347:THR:N	2.70	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: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:B:468:PRO:HG2	1:B:471:ASN:CG	2.39	0.47
1:C:339:ASP:OD1	1:C:339:ASP:N	2.48	0.47
1:B:345:LEU:C	1:B:347:THR:H	2.23	0.47
1:D:484:PHE:HB3	1:D:515:MET:HE1	1.96	0.47
1:C:336:VAL:O	1:C:381:ALA:HB2	2.14	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: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:D:316:ALA:HB1	1:D:322:PHE:HB2	1.97	0.46
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:A:484:PHE:CD1	1:A:515:MET:HE1	2.52	0.45
1:B:450:GLN:O	1:B:453:PRO:HD2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:355:PHE:HZ	1:B:380:LEU:HD23	1.82	0.44
1:A:496:VAL:O	1:A:496:VAL:HG23	2.17	0.44
1:D:325:LEU:C	1:D:327:ASP:N	2.75	0.44
1:A:303:ARG:HG2	1:A:307:MET:HE3	1.98	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:D:481:GLU:CD	1:D:512:LYS:HD2	2.42	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:510:ALA:HA	1:A:515:MET:HE3	2.00	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:C:470:GLU:CD	1:C:470:GLU:H	2.24	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: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: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:315:LEU:C	1:C:315:LEU:CD2	2.92	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:D:315:LEU:HD23	1:D:315:LEU:C	2.43	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:C:480:LYS:HZ2	1:C:506:GLU:HG2	1.81	0.42
1:D:350:PHE:CD2	1:D:383:ARG:HD3	2.54	0.42
1:B:536:GLU:C	1:B:538:LEU:N	2.77	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:ASP:OD1	1:D:377:MET:HE3	2.18	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:C:404:THR:HG23	1:C:405:PRO:HA	2.01	0.42
1:D:470:GLU:CD	1:D:470:GLU:H	2.27	0.42
1:B:331:ILE:HD11	1:B:478:THR:HG21	2.01	0.42
1:C:311:MET:HE1	1:C:410:TRP:HB2	2.00	0.42
1:B:315:LEU:HD12	1:B:402:ILE:HD11	2.02	0.42
1:B:339:ASP:CG	1:B:377:MET:HE3	2.45	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:C:475:ALA:HB1	1:C:479:GLY:C	2.45	0.41
1:A:343:GLN:O	1:A:385:ARG:NH2	2.45	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:B:311:MET:CE	1:B:413:LEU:HD23	2.48	0.41
1:A:504:VAL:HG23	1:A:505:GLU:N	2.35	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:A:468:PRO:HG2	1:A:471:ASN:CG	2.47	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:B:311:MET:HE2	1:B:413:LEU:HD22	2.03	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:B:315:LEU:C	1:B:315:LEU:HD23	2.47	0.40
1:D:514:ASN:N	1:D:514:ASN:HD22	2.18	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	30	49
1	B	249/274 (91%)	233 (94%)	11 (4%)	5 (2%)	6	10
1	C	255/274 (93%)	234 (92%)	18 (7%)	3 (1%)	10	20
1	D	252/274 (92%)	233 (92%)	15 (6%)	4 (2%)	7	14
All	All	1011/1096 (92%)	943 (93%)	55 (5%)	13 (1%)	9	18

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%)	216 (95%)	11 (5%)	23	46
1	B	223/237 (94%)	210 (94%)	13 (6%)	18	38
1	C	227/237 (96%)	212 (93%)	15 (7%)	15	32
1	D	224/237 (94%)	216 (96%)	8 (4%)	31	58
All	All	901/948 (95%)	854 (95%)	47 (5%)	21	42

All (47) 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	402	ILE
1	A	423	LEU
1	A	490	ARG
1	A	493	ARG
1	A	506	GLU
1	A	530	ARG
1	B	268	GLU
1	B	326	GLU
1	B	333	VAL
1	B	341	ASN
1	B	378	ARG
1	B	380	LEU
1	B	412	GLN
1	B	414	ARG
1	B	448	THR
1	B	506	GLU
1	B	526	LEU
1	B	529	LEU
1	B	530	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	266	HIS
1	C	315	LEU
1	C	329	ASP
1	C	330	GLN
1	C	339	ASP
1	C	353	ASP
1	C	356	HIS
1	C	382	PHE
1	C	402	ILE
1	C	417	LEU
1	C	466	VAL
1	C	470	GLU
1	C	490	ARG
1	C	506	GLU
1	C	514	ASN
1	D	330	GLN
1	D	339	ASP
1	D	386	ARG
1	D	414	ARG
1	D	470	GLU
1	D	476	THR
1	D	506	GLU
1	D	526	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	HIS
1	A	314	ASN
1	A	319	HIS
1	A	330	GLN
1	A	343	GLN
1	A	349	ASN
1	A	412	GLN
1	A	427	HIS
1	A	436	ASN
1	A	450	GLN
1	A	508	GLN
1	A	513	HIS
1	B	283	HIS
1	B	319	HIS
1	B	330	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	341	ASN
1	B	412	GLN
1	B	427	HIS
1	B	450	GLN
1	B	523	HIS
1	B	531	HIS
1	C	266	HIS
1	C	319	HIS
1	C	341	ASN
1	C	396	ASN
1	C	412	GLN
1	C	450	GLN
1	D	341	ASN
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 oligosaccharides 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	D	804	1	0,3,3	-	-	-		
2	BEF	B	802	1	0,3,3	-	-	-		
2	BEF	C	803	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

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, 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%)	-0.07	8 (3%) 51 47	26, 37, 61, 78	0
1	B	253/274 (92%)	0.48	31 (12%) 8 7	28, 48, 80, 80	0
1	C	259/274 (94%)	0.45	26 (10%) 12 10	31, 48, 80, 80	0
1	D	256/274 (93%)	0.27	21 (8%) 17 15	28, 44, 80, 80	0
All	All	1027/1096 (93%)	0.28	86 (8%) 17 15	26, 44, 80, 80	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	356	HIS	5.9
1	D	356	HIS	5.7
1	C	356	HIS	5.1
1	C	374	VAL	4.9
1	B	354	GLY	4.9
1	A	356	HIS	4.9
1	B	342	GLY	4.8
1	A	372	GLY	4.7
1	A	374	VAL	4.4
1	B	355	PHE	4.2
1	C	344	ASP	4.1
1	B	329	ASP	4.0
1	C	372	GLY	3.8
1	B	379	LYS	3.7
1	C	336	VAL	3.5
1	C	337	SER	3.4
1	C	265	SER	3.4
1	B	337	SER	3.3
1	B	347	THR	3.3
1	A	265	SER	3.2
1	D	354	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	337	SER	3.1
1	A	373	GLY	3.1
1	D	374	VAL	3.0
1	C	347	THR	3.0
1	B	344	ASP	3.0
1	B	378	ARG	3.0
1	C	354	GLY	3.0
1	C	329	ASP	2.9
1	B	338	SER	2.9
1	D	338	SER	2.8
1	B	376	TRP	2.8
1	B	328	CYS	2.8
1	C	313	PHE	2.8
1	C	376	TRP	2.8
1	C	328	CYS	2.8
1	C	373	GLY	2.8
1	D	372	GLY	2.8
1	B	346	SER	2.7
1	C	341	ASN	2.7
1	D	378	ARG	2.7
1	C	355	PHE	2.7
1	B	494	LYS	2.7
1	C	338	SER	2.7
1	B	352	ALA	2.7
1	B	343	GLN	2.7
1	A	375	ASP	2.6
1	B	375	ASP	2.6
1	D	328	CYS	2.6
1	C	345	LEU	2.6
1	D	327	ASP	2.6
1	B	348	TYR	2.6
1	B	402	ILE	2.6
1	D	376	TRP	2.6
1	B	341	ASN	2.6
1	B	336	VAL	2.5
1	D	343	GLN	2.5
1	C	351	SER	2.5
1	D	341	ASN	2.4
1	B	489	GLN	2.4
1	C	402	ILE	2.3
1	C	375	ASP	2.3
1	C	352	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	336	VAL	2.3
1	D	404	THR	2.3
1	B	380	LEU	2.3
1	D	477	LYS	2.3
1	A	355	PHE	2.3
1	B	333	VAL	2.3
1	D	355	PHE	2.2
1	D	342	GLY	2.2
1	C	346	SER	2.2
1	D	347	THR	2.2
1	D	352	ALA	2.2
1	C	327	ASP	2.2
1	D	373	GLY	2.1
1	C	348	TYR	2.1
1	B	339	ASP	2.1
1	B	345	LEU	2.1
1	B	377	MET	2.1
1	B	382	PHE	2.1
1	B	393	THR	2.1
1	C	494	LYS	2.1
1	B	340	ASP	2.0
1	D	345	LEU	2.0
1	A	512	LYS	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 oligosaccharides 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.

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
-----	------	-------	-----	-------	------	-----	-----------------------------	-------

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	701	1/1	0.86	0.07	36,36,36,36	0
3	MG	B	702	1/1	0.89	0.08	44,44,44,44	0
3	MG	D	704	1/1	0.90	0.10	43,43,43,43	0
2	BEF	C	803	4/4	0.91	0.10	40,40,41,41	0
2	BEF	D	804	4/4	0.93	0.07	35,36,37,39	0
2	BEF	B	802	4/4	0.93	0.08	43,43,44,44	0
3	MG	C	703	1/1	0.94	0.06	39,39,39,39	0
2	BEF	A	801	4/4	0.96	0.07	33,33,34,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.