



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:51 AM UTC

PDB ID : 1XVG / pdb_00001xvg
Title : soluble methane monooxygenase hydroxylase: bromoethanol soaked structure
Authors : Sazinsky, M.H.; Lippard, S.J.
Deposited on : 2004-10-27
Resolution : 1.96 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:

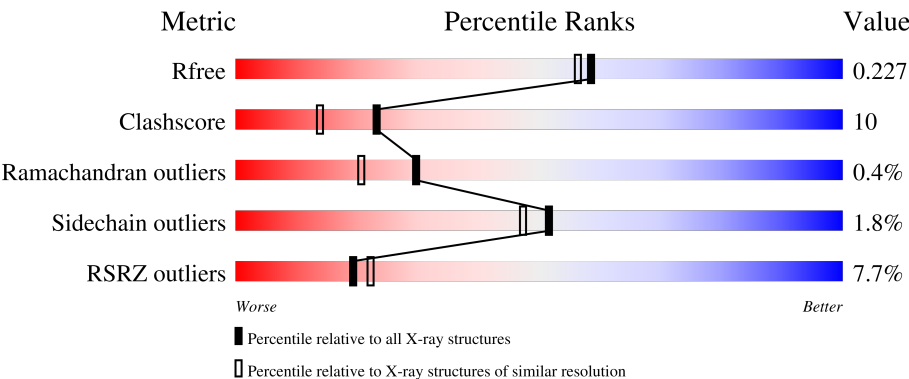
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	527	4% 72% 22% ..
1	B	527	3% 72% 24% ..
2	C	389	2% 81% 19% .
2	D	389	13% 75% 22% .
3	E	170	4% 78% 19% ..

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Mol	Chain	Length	Quality of chain
3	F	170	39% 61% 34% • •

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18633 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 Methane monooxygenase component A alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			4148	2655	713	762	18			
1	B	510	Total	C	N	O	S	0	0	0
			4137	2646	711	762	18			

- Molecule 2 is a protein called Methane monooxygenase component A beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	388	Total	C	N	O	S	0	0	0
			3163	2036	545	574	8			
2	D	388	Total	C	N	O	S	0	0	0
			3151	2028	543	572	8			

- Molecule 3 is a protein called Methane monooxygenase component A gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	166	Total	C	N	O	S	0	0	0
			1364	864	245	250	5			
3	F	166	Total	C	N	O	S	0	0	0
			1358	860	243	250	5			

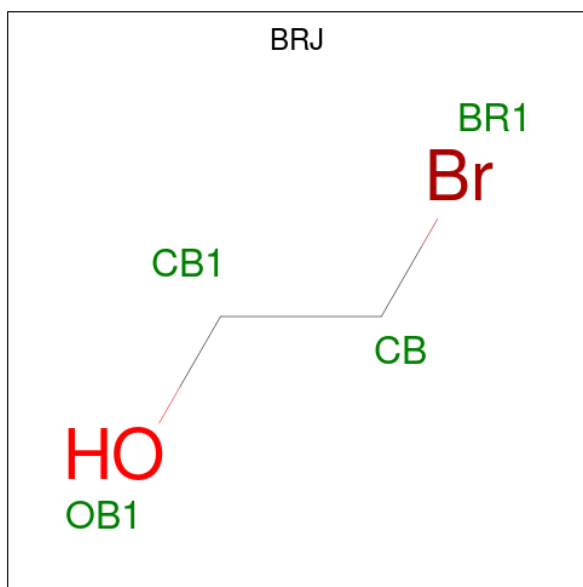
- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Fe	0	0
			2	2		
4	B	2	Total	Fe	0	0
			2	2		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	C	3	Total Ca 3 3	0	0

- Molecule 6 is 2-BROMOETHANOL (CCD ID: BRJ) (formula: C₂H₅BrO).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Br C O 4 1 2 1	0	0
6	A	1	Total Br C O 4 1 2 1	0	0
6	A	1	Total Br C O 4 1 2 1	0	0
6	A	1	Total Br C O 4 1 2 1	0	0
6	B	1	Total Br C O 4 1 2 1	0	0
6	B	1	Total Br C O 4 1 2 1	0	0
6	B	1	Total Br C O 4 1 2 1	0	0
6	B	1	Total Br C O 4 1 2 1	0	0
6	C	1	Total Br C O 4 1 2 1	0	0
6	C	1	Total Br C O 4 1 2 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total 4	Br 1	C 2	O 1	0	0
6	C	1	Total 4	Br 1	C 2	O 1	0	0

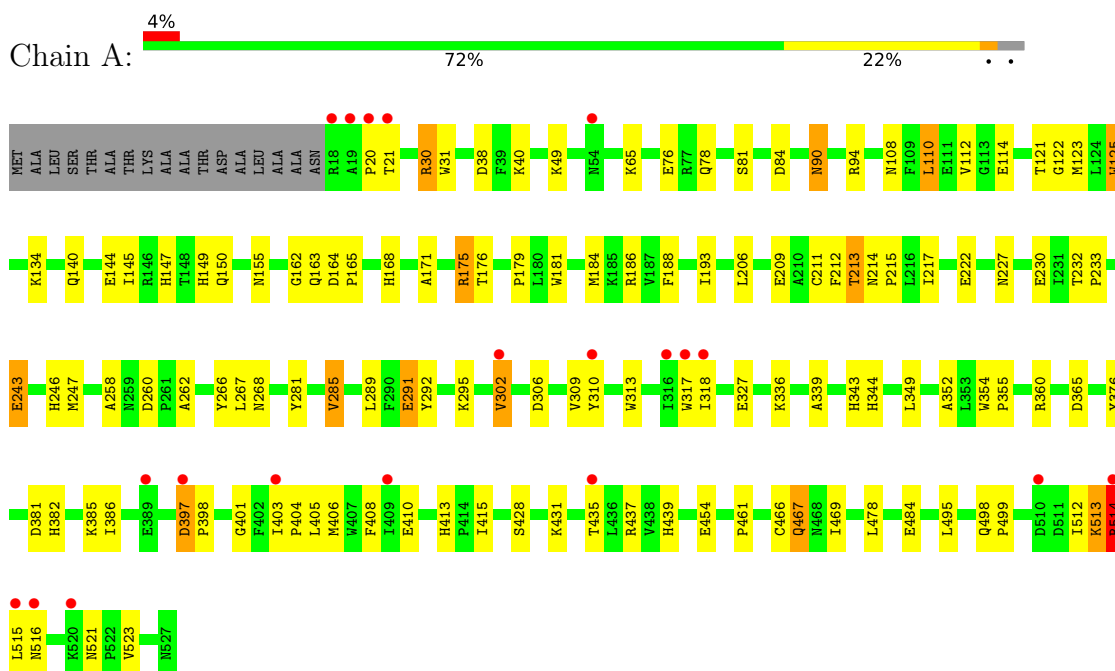
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	313	Total 313	O 313	0	0
7	B	278	Total 278	O 278	0	0
7	C	280	Total 280	O 280	0	0
7	D	167	Total 167	O 167	0	0
7	E	153	Total 153	O 153	0	0
7	F	65	Total 65	O 65	0	0

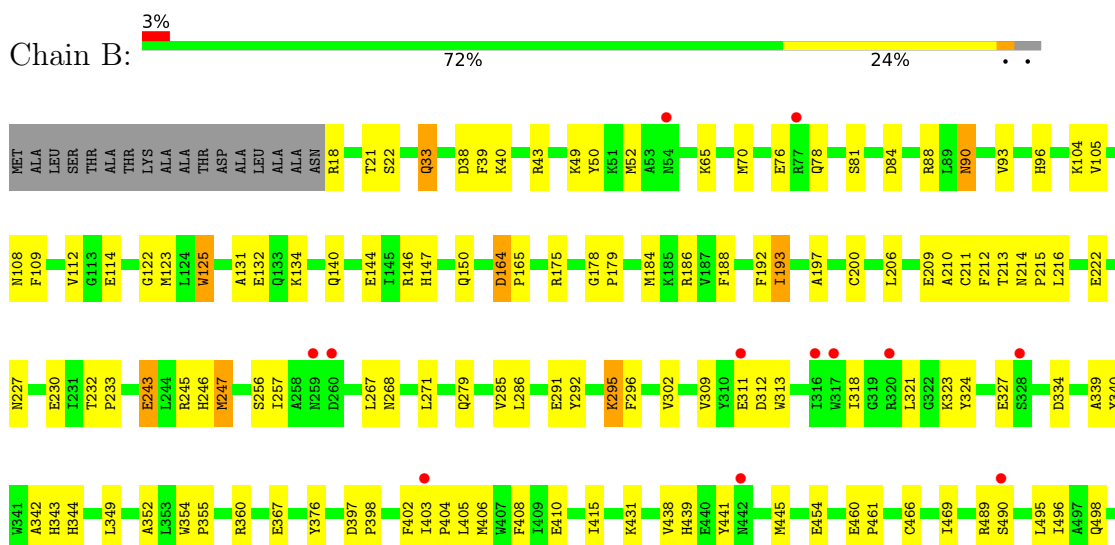
3 Residue-property plots [i](#)

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: Methane monooxygenase component A alpha chain

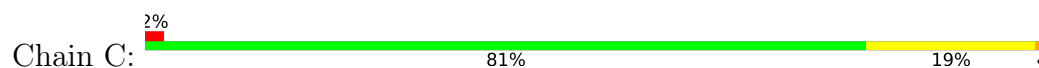


- Molecule 1: Methane monooxygenase component A alpha chain

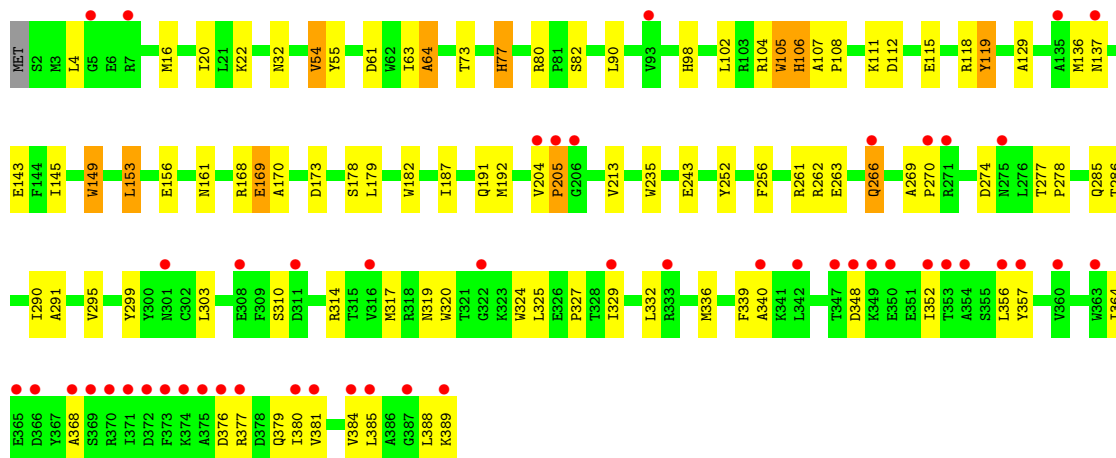
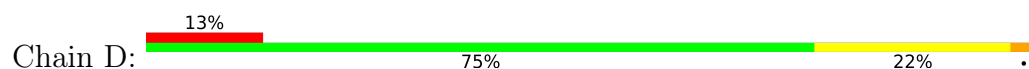




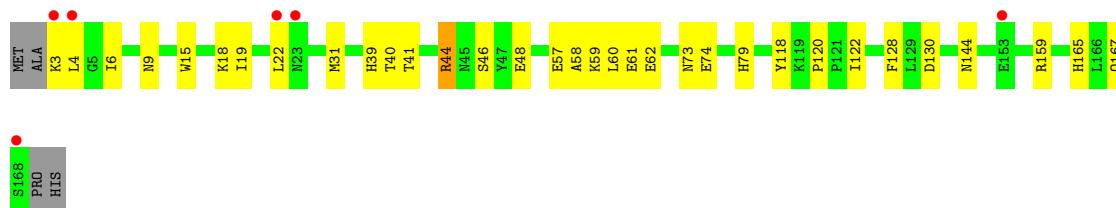
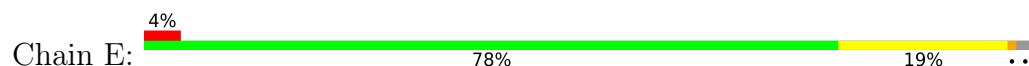
- Molecule 2: Methane monooxygenase component A beta chain



- Molecule 2: Methane monooxygenase component A beta chain

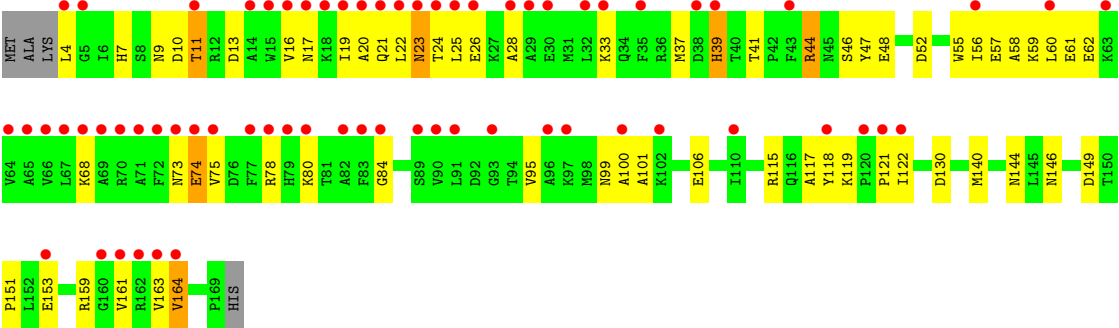


- Molecule 3: Methane monooxygenase component A gamma chain



- Molecule 3: Methane monooxygenase component A gamma chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.28Å 171.54Å 221.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 1.96 29.97 – 1.96	Depositor EDS
% Data completeness (in resolution range)	93.1 (29.97-1.96) 93.1 (29.97-1.96)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 1.95Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.198 , 0.230 0.195 , 0.227	Depositor DCC
R_{free} test set	9060 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18633	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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: CA, BRJ, FE

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	0.41	0/4273	0.96	28/5808 (0.5%)
1	B	0.37	0/4262	0.90	22/5796 (0.4%)
2	C	0.39	0/3259	0.88	17/4430 (0.4%)
2	D	0.35	0/3247	0.84	13/4417 (0.3%)
3	E	0.39	0/1392	0.89	7/1876 (0.4%)
3	F	0.32	0/1387	0.81	4/1873 (0.2%)
All	All	0.38	0/17820	0.89	91/24200 (0.4%)

There are no bond length outliers.

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	339	ALA	N-CA-C	9.31	121.19	111.14
1	A	516	ASN	CA-C-O	8.81	131.91	120.98
1	A	164	ASP	CA-C-N	8.74	128.46	119.19
1	A	164	ASP	C-N-CA	8.74	128.46	119.19
1	A	513	LYS	N-CA-C	7.76	120.42	111.11
1	A	516	ASN	O-C-N	-7.63	112.40	122.47
1	A	339	ALA	N-CA-C	7.57	119.61	111.36
1	A	309	VAL	N-CA-C	7.32	117.41	110.53
3	E	130	ASP	N-CA-C	-7.26	103.44	111.36
2	C	106	HIS	N-CA-C	6.81	118.70	111.28
1	B	285	VAL	N-CA-C	6.75	116.90	110.42
1	A	212	PHE	N-CA-C	6.74	121.37	112.13
2	D	105	TRP	N-CA-C	-6.57	100.49	109.95
1	B	431	LYS	N-CA-C	-6.47	105.21	113.23
1	B	243	GLU	N-CA-C	6.37	119.03	111.71
2	C	236	GLN	N-CA-C	6.36	121.20	113.38
1	B	309	VAL	N-CA-C	6.32	116.36	110.42
2	C	169	GLU	N-CA-C	6.25	120.90	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	377	ARG	N-CA-C	6.21	118.05	111.28
1	A	516	ASN	OD1-CG-ND2	-6.19	116.41	122.60
1	A	266	TYR	N-CA-C	6.16	121.68	114.04
1	A	145	ILE	N-CA-C	-6.15	104.51	110.72
1	B	496	ILE	N-CA-C	-6.14	104.76	110.53
1	A	285	VAL	N-CA-C	6.12	116.28	110.53
2	C	149	TRP	N-CA-C	-6.10	104.71	111.36
1	B	295	LYS	N-CA-C	-6.08	103.80	112.13
2	D	204	VAL	CA-C-N	6.07	127.43	119.84
2	D	204	VAL	C-N-CA	6.07	127.43	119.84
1	A	397	ASP	CA-C-N	6.06	125.94	119.28
1	A	397	ASP	C-N-CA	6.06	125.94	119.28
1	A	243	GLU	N-CA-C	5.99	118.60	111.71
3	E	79	HIS	N-CA-C	5.91	121.22	113.30
2	D	106	HIS	N-CA-C	5.90	118.19	111.11
3	F	39	HIS	N-CA-C	5.88	121.78	113.02
1	B	93	VAL	N-CA-C	5.86	116.85	111.81
1	B	212	PHE	N-CA-C	5.85	120.14	112.13
3	F	118	TYR	N-CA-C	5.84	120.41	112.88
1	A	122	GLY	N-CA-C	-5.78	105.37	112.77
1	B	122	GLY	N-CA-C	-5.78	105.38	112.77
2	C	252	TYR	N-CA-C	5.77	117.26	110.97
2	D	119	TYR	N-CA-C	-5.76	105.00	111.28
3	E	118	TYR	N-CA-C	5.74	120.99	113.30
2	C	262	ARG	N-CA-C	5.73	118.73	111.69
2	C	53	THR	N-CA-C	5.72	119.96	112.13
2	C	105	TRP	N-CA-C	-5.64	101.08	109.94
2	D	149	TRP	N-CA-C	-5.64	105.21	111.36
1	A	478	LEU	N-CA-C	5.63	117.87	111.11
1	B	104	LYS	N-CA-C	-5.61	105.25	111.36
1	B	340	TYR	N-CA-C	5.60	120.56	111.37
2	C	56	ALA	N-CA-C	-5.56	105.30	111.36
3	E	39	HIS	N-CA-C	5.54	121.92	113.61
1	A	431	LYS	N-CA-C	-5.47	106.45	113.23
1	B	312	ASP	N-CA-C	5.41	116.86	110.97
2	C	54	VAL	N-CA-C	5.38	116.63	109.37
2	C	265	PHE	N-CA-C	5.37	116.82	111.07
3	E	122	ILE	N-CA-C	-5.35	105.87	110.74
3	E	73	ASN	N-CA-C	-5.35	102.97	110.35
1	B	193	ILE	N-CA-C	5.35	120.46	109.34
2	D	104	ARG	N-CA-C	5.33	117.44	108.96
2	C	299	TYR	N-CA-C	5.32	118.94	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	513	LYS	CA-C-O	-5.30	115.22	120.90
1	B	247	MET	N-CA-C	-5.30	105.40	111.07
1	B	65	LYS	N-CA-C	5.30	117.06	111.28
1	B	342	ALA	N-CA-C	5.28	117.45	111.11
2	C	104	ARG	N-CA-C	5.27	116.89	108.41
3	F	130	ASP	N-CA-C	-5.25	105.63	111.36
3	E	74	GLU	N-CA-C	5.22	116.97	111.28
2	D	54	VAL	N-CA-C	5.20	116.39	109.37
1	B	178	GLY	CA-C-N	5.20	124.70	119.19
1	B	178	GLY	C-N-CA	5.20	124.70	119.19
3	F	75	VAL	N-CA-C	5.19	115.40	110.42
2	D	137	ASN	CA-C-N	5.17	124.61	119.24
2	D	137	ASN	C-N-CA	5.17	124.61	119.24
1	B	164	ASP	CA-C-N	5.16	124.96	119.28
1	B	164	ASP	C-N-CA	5.16	124.96	119.28
1	B	267	LEU	N-CA-C	5.14	117.29	111.02
2	D	77	HIS	N-CA-C	-5.13	102.45	110.10
2	C	63	ILE	N-CA-C	-5.12	98.57	106.72
1	A	267	LEU	N-CA-C	5.09	117.23	111.02
1	A	213	THR	N-CA-C	5.09	116.51	111.07
1	A	291	GLU	N-CA-C	5.08	116.90	111.36
2	D	252	TYR	N-CA-C	5.06	116.49	110.97
1	A	162	GLY	N-CA-C	5.05	120.56	112.58
1	A	193	ILE	N-CA-C	5.04	119.83	109.34
2	C	249	HIS	N-CA-C	5.04	118.58	112.23
1	A	513	LYS	O-C-N	-5.03	116.86	122.09
1	A	514	ARG	CA-C-N	5.02	127.42	120.29
1	A	514	ARG	C-N-CA	5.02	127.42	120.29
2	C	77	HIS	N-CA-C	-5.02	102.62	110.10
2	D	169	GLU	N-CA-C	5.02	119.46	113.23
1	A	258	ALA	N-CA-C	5.02	116.75	111.28

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	4148	0	3919	97	0
1	B	4137	0	3888	107	0
2	C	3163	0	2986	48	0
2	D	3151	0	2960	73	0
3	E	1364	0	1352	19	0
3	F	1358	0	1335	47	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	C	3	0	0	0	0
6	A	16	0	11	1	0
6	B	16	0	11	0	0
6	C	16	0	12	2	0
7	A	313	0	0	6	0
7	B	278	0	0	9	0
7	C	280	0	0	5	0
7	D	167	0	0	4	0
7	E	153	0	0	1	0
7	F	65	0	0	1	0
All	All	18633	0	16474	349	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 10.

All (349) 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)
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.38	1.03
3:F:80:LYS:HE2	3:F:84:GLY:HA2	1.40	1.00
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.11	0.94
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.09	0.92
3:F:41:THR:O	3:F:44:ARG:HD2	1.76	0.86
1:B:268:ASN:HD21	1:B:327:GLU:H	1.22	0.85
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.57	0.84
1:A:435:THR:CG2	1:A:437:ARG:HE	1.92	0.82
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.61	0.82
2:D:340:ALA:HA	2:D:389:LYS:HE2	1.62	0.82
1:A:467:GLN:HG3	7:A:3809:HOH:O	1.78	0.81
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.64	0.80
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.30	0.80
1:A:313:TRP:CE2	1:A:318:ILE:HD11	2.17	0.79
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:PRO:HG2	1:A:403:ILE:HD13	1.65	0.78
1:A:289:LEU:HD23	6:A:3805:BRJ:BR1	2.39	0.77
1:A:268:ASN:HD21	1:A:327:GLU:H	1.31	0.77
3:E:41:THR:O	3:E:44:ARG:HD2	1.84	0.76
1:B:209:GLU:HA	1:B:213:THR:OG1	1.85	0.76
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.67	0.75
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.33	0.75
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.34	0.74
3:F:13:ASP:O	3:F:16:VAL:HG22	1.87	0.74
1:A:213:THR:O	1:A:217:ILE:HG12	1.89	0.73
1:B:33:GLN:HE22	1:B:132:GLU:H	1.34	0.73
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.86	0.72
1:B:108:ASN:HD21	1:B:175:ARG:HH11	1.36	0.72
1:A:406:MET:O	1:A:410:GLU:HG3	1.90	0.71
3:F:19:ILE:HD12	3:F:20:ALA:N	2.05	0.71
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.71	0.71
2:D:348:ASP:O	2:D:352:ILE:HG12	1.91	0.70
1:A:435:THR:HG21	1:A:437:ARG:HE	1.55	0.70
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.21	0.70
1:B:123:MET:HE3	1:B:197:ALA:HA	1.73	0.70
2:D:325:LEU:O	2:D:329:ILE:HG12	1.91	0.70
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.74	0.70
3:F:4:LEU:HD11	3:F:10:ASP:OD2	1.92	0.69
3:F:52:ASP:O	3:F:56:ILE:HG12	1.93	0.69
1:A:227:ASN:HD21	1:A:295:LYS:H	1.39	0.69
1:B:125:TRP:HE1	2:D:161:ASN:ND2	1.90	0.69
1:A:20:PRO:HG3	2:C:129:ALA:HB2	1.73	0.68
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.41	0.67
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.96	0.66
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.60	0.66
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.77	0.66
1:B:88:ARG:NH1	7:B:4055:HOH:O	2.10	0.66
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.25	0.66
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.78	0.65
3:F:9:ASN:OD1	3:F:11:THR:HG23	1.95	0.65
1:B:33:GLN:NE2	1:B:132:GLU:H	1.94	0.65
2:C:318:ARG:NH2	7:C:4078:HOH:O	2.30	0.65
1:B:123:MET:HE1	1:B:200:CYS:SG	2.37	0.65
2:D:291:ALA:O	2:D:295:VAL:HG23	1.98	0.64
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.32	0.64
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:TRP:HE1	2:D:161:ASN:HD22	1.46	0.62
1:A:230:GLU:HB3	7:B:4055:HOH:O	1.99	0.62
1:A:306:ASP:HB2	7:A:4104:HOH:O	1.99	0.62
1:B:268:ASN:ND2	1:B:327:GLU:H	1.94	0.62
3:F:153:GLU:H	3:F:153:GLU:CD	2.07	0.62
3:E:165:HIS:HE1	3:E:167:GLN:NE2	1.97	0.62
1:B:349:LEU:HD22	1:B:415:ILE:HD12	1.82	0.62
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.81	0.62
1:A:175:ARG:HG3	1:A:181:TRP:CD2	2.34	0.62
3:E:165:HIS:HE1	3:E:167:GLN:HE21	1.47	0.62
1:A:184:MET:HE2	1:A:188:PHE:CG	2.35	0.61
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.97	0.61
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.84	0.61
1:B:33:GLN:HE21	1:B:33:GLN:HA	1.65	0.60
3:E:58:ALA:O	3:E:62:GLU:HG3	2.00	0.60
1:B:88:ARG:NE	7:B:4061:HOH:O	2.24	0.60
3:F:57:GLU:O	3:F:61:GLU:HG3	2.01	0.60
1:B:438:VAL:HB	3:F:164:VAL:HG22	1.83	0.60
1:A:513:LYS:O	1:A:514:ARG:C	2.44	0.60
2:C:209:GLU:HG2	7:C:3843:HOH:O	2.01	0.59
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.83	0.59
1:A:382:HIS:O	1:A:386:ILE:HG12	2.02	0.59
1:B:96:HIS:HB2	2:D:20:ILE:HD12	1.85	0.59
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.83	0.59
1:A:313:TRP:O	1:A:318:ILE:HD13	2.03	0.59
1:B:70:MET:HE1	1:B:245:ARG:NH1	2.17	0.59
1:B:184:MET:HE2	1:B:188:PHE:CG	2.38	0.59
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.84	0.58
3:F:33:LYS:O	3:F:37:MET:HG2	2.02	0.58
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.33	0.58
2:D:256:PHE:HA	2:D:332:LEU:HD21	1.85	0.58
1:A:349:LEU:HD22	1:A:415:ILE:HD12	1.84	0.58
1:A:401:GLY:HA2	1:A:515:LEU:CD2	2.33	0.58
3:F:80:LYS:HE2	3:F:84:GLY:CA	2.24	0.58
3:F:58:ALA:O	3:F:62:GLU:HG3	2.04	0.58
3:E:4:LEU:O	3:E:4:LEU:HG	2.04	0.57
1:A:413:HIS:HD2	1:A:428:SER:OG	1.87	0.57
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.39	0.57
2:D:143:GLU:HG2	7:D:555:HOH:O	2.04	0.57
1:B:184:MET:HE2	1:B:188:PHE:CD2	2.39	0.57
3:E:165:HIS:CE1	3:E:167:GLN:HE21	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ASN:HD21	1:B:295:LYS:H	1.51	0.57
1:B:489:ARG:HD2	1:B:495:LEU:O	2.03	0.57
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.88	0.57
2:D:153:LEU:C	2:D:153:LEU:HD12	2.30	0.57
3:F:25:LEU:HD22	3:F:68:LYS:HA	1.87	0.57
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.40	0.56
1:B:398:PRO:HG3	1:B:507:TRP:CD1	2.40	0.56
2:D:324:TRP:C	2:D:327:PRO:HD2	2.29	0.56
3:F:22:LEU:HD13	3:F:28:ALA:HA	1.86	0.56
3:E:41:THR:O	3:E:44:ARG:CD	2.52	0.56
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.88	0.56
2:C:333:ARG:HD2	7:C:3935:HOH:O	2.04	0.56
1:B:439:HIS:HE1	1:B:454:GLU:OE1	1.88	0.55
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.88	0.55
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.72	0.55
2:D:261:ARG:HE	2:D:285:GLN:NE2	2.05	0.55
3:F:61:GLU:O	3:F:121:PRO:HG2	2.07	0.55
1:A:268:ASN:ND2	1:A:327:GLU:H	2.01	0.55
1:B:403:ILE:HD11	1:B:507:TRP:CZ3	2.41	0.55
1:B:405:LEU:HD11	7:B:4078:HOH:O	2.05	0.55
1:A:227:ASN:ND2	1:A:295:LYS:H	2.05	0.54
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.38	0.54
2:D:187:ILE:O	2:D:191:GLN:HG3	2.06	0.54
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.71	0.54
1:B:184:MET:HE3	1:B:184:MET:HA	1.89	0.54
1:A:184:MET:HE3	1:A:184:MET:HA	1.88	0.54
3:E:57:GLU:O	3:E:61:GLU:HG3	2.08	0.54
1:A:209:GLU:HA	1:A:213:THR:OG1	2.08	0.54
2:C:2:SER:HB2	7:C:4067:HOH:O	2.08	0.54
2:D:381:VAL:O	2:D:385:LEU:HB2	2.08	0.53
3:E:22:LEU:HD11	3:E:31:MET:SD	2.48	0.53
6:C:3808:BRJ:HB12	2:D:286:THR:OG1	2.08	0.53
1:B:490:SER:OG	2:D:32:ASN:HB2	2.08	0.53
1:B:445:MET:HE3	1:B:523:VAL:HG22	1.90	0.53
1:B:367:GLU:HG3	7:B:4026:HOH:O	2.07	0.53
2:C:98:HIS:HE1	2:C:178:SER:OG	1.92	0.53
1:B:123:MET:HB2	2:D:168:ARG:HD3	1.91	0.53
2:D:192:MET:HA	2:D:192:MET:HE2	1.91	0.53
1:B:108:ASN:ND2	1:B:175:ARG:HH11	2.05	0.52
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.27	0.52
3:F:33:LYS:HE3	3:F:117:ALA:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:39:HIS:HD2	7:F:175:HOH:O	1.91	0.52
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.44	0.52
1:B:402:PHE:C	1:B:403:ILE:HD12	2.33	0.52
2:C:211:THR:O	2:C:214:PRO:HD2	2.09	0.52
2:D:340:ALA:HB2	2:D:389:LYS:HG2	1.92	0.52
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.75	0.52
1:A:175:ARG:HG2	1:A:176:THR:N	2.24	0.51
1:A:484:GLU:OE1	3:E:6:ILE:N	2.38	0.51
1:A:495:LEU:HD11	1:A:512:ILE:HG13	1.93	0.51
3:F:23:ASN:H	3:F:23:ASN:HD22	1.58	0.51
3:F:46:SER:OG	3:F:48:GLU:HG2	2.10	0.51
1:A:123:MET:HB2	2:C:168:ARG:HD3	1.92	0.51
1:A:408:PHE:CD2	1:A:415:ILE:HD11	2.45	0.51
2:C:143:GLU:O	2:C:147:ARG:HB3	2.10	0.51
2:D:111:LYS:O	2:D:115:GLU:HG3	2.11	0.51
3:F:115:ARG:O	3:F:119:LYS:HB2	2.10	0.51
1:A:84:ASP:HB3	1:B:81:SER:OG	2.10	0.51
1:B:243:GLU:O	1:B:247:MET:HG2	2.11	0.51
1:B:406:MET:O	1:B:410:GLU:HG3	2.10	0.51
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.92	0.50
1:A:140:GLN:O	1:A:144:GLU:HG2	2.11	0.50
1:A:260:ASP:OD2	1:A:262:ALA:HB3	2.12	0.50
2:D:310:SER:O	2:D:314:ARG:HG3	2.11	0.50
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.93	0.50
1:A:76:GLU:HG2	1:B:76:GLU:OE2	2.11	0.50
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.94	0.50
2:D:105:TRP:O	2:D:108:PRO:HD2	2.11	0.50
2:C:235:TRP:CD1	2:C:235:TRP:C	2.90	0.50
3:F:19:ILE:HD12	3:F:19:ILE:C	2.37	0.50
1:A:108:ASN:HD21	1:A:175:ARG:HE	1.57	0.50
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.94	0.50
1:B:461:PRO:HG2	3:F:159:ARG:CZ	2.41	0.50
2:D:54:VAL:O	2:D:55:TYR:HB2	2.12	0.50
2:C:153:LEU:C	2:C:153:LEU:HD12	2.37	0.49
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.44	0.49
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.77	0.49
1:B:403:ILE:HG22	1:B:405:LEU:H	1.77	0.49
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.12	0.49
3:E:46:SER:OG	3:E:48:GLU:HG2	2.12	0.49
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.94	0.49
1:B:164:ASP:CG	1:B:489:ARG:HH22	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.46	0.49
1:B:186:ARG:HA	2:D:73:THR:OG1	2.12	0.49
2:D:16:MET:O	2:D:20:ILE:HG12	2.12	0.49
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.95	0.49
2:D:357:TYR:CE2	2:D:381:VAL:HG21	2.48	0.49
2:D:277:THR:HB	2:D:278:PRO:HD3	1.95	0.49
1:B:403:ILE:HD13	1:B:515:LEU:HD13	1.94	0.49
1:A:163:GLN:HG2	7:A:4012:HOH:O	2.12	0.48
1:A:184:MET:HE2	1:A:188:PHE:CD2	2.47	0.48
1:B:186:ARG:HD3	1:B:186:ARG:C	2.38	0.48
1:B:521:ASN:OD1	1:B:523:VAL:HG12	2.13	0.48
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.48	0.48
2:D:213:VAL:HG23	7:D:418:HOH:O	2.14	0.48
1:A:246:HIS:N	1:A:246:HIS:CD2	2.81	0.48
1:A:521:ASN:OD1	1:A:523:VAL:HG12	2.13	0.48
1:B:247:MET:HE2	1:B:247:MET:HA	1.95	0.48
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.48	0.48
3:F:146:ASN:HB3	3:F:149:ASP:OD2	2.13	0.48
3:F:73:ASN:O	3:F:74:GLU:C	2.57	0.48
1:B:210:ALA:N	1:B:247:MET:HE1	2.29	0.48
1:B:408:PHE:CD2	1:B:415:ILE:HD11	2.49	0.48
3:E:15:TRP:CZ3	3:E:18:LYS:HD3	2.49	0.48
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.11	0.48
1:B:18:ARG:O	2:D:129:ALA:HA	2.14	0.48
1:B:49:LYS:HD3	3:F:144:ASN:HD22	1.79	0.48
2:D:356:LEU:HD12	2:D:385:LEU:HD13	1.96	0.47
3:F:17:ASN:O	3:F:21:GLN:HG2	2.14	0.47
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.49	0.47
1:A:317:TRP:HD1	1:A:318:ILE:HD12	1.80	0.47
1:B:43:ARG:HD2	1:B:43:ARG:C	2.39	0.47
1:A:81:SER:OG	1:B:84:ASP:HB3	2.14	0.47
1:A:186:ARG:HA	2:C:73:THR:OG1	2.15	0.47
1:B:441:TYR:HB2	3:F:161:VAL:HG23	1.97	0.47
2:C:146:ASN:ND2	2:C:197:ARG:HH21	2.08	0.47
2:C:146:ASN:O	2:C:214:PRO:HG3	2.14	0.47
1:B:33:GLN:HA	1:B:131:ALA:HB3	1.97	0.47
1:B:88:ARG:NH2	7:B:4061:HOH:O	2.47	0.47
1:B:144:GLU:OE2	1:B:144:GLU:HA	2.15	0.47
2:D:339:PHE:CZ	2:D:352:ILE:HD12	2.49	0.47
6:C:3807:BRJ:CB	2:D:119:TYR:CZ	2.97	0.47
2:D:376:ASP:OD1	2:D:379:GLN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:TYR:CZ	1:A:285:VAL:HG21	2.50	0.47
1:B:227:ASN:ND2	1:B:295:LYS:H	2.11	0.47
2:D:98:HIS:HE1	2:D:178:SER:OG	1.98	0.47
2:D:77:HIS:CG	3:F:140:MET:HG2	2.50	0.46
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.15	0.46
1:A:125:TRP:HE1	2:C:161:ASN:HD22	1.63	0.46
1:A:175:ARG:HG3	1:A:181:TRP:CE2	2.50	0.46
2:D:235:TRP:CD1	2:D:235:TRP:C	2.93	0.46
1:B:140:GLN:O	1:B:144:GLU:HG2	2.15	0.46
1:B:466:CYS:HB2	2:D:73:THR:HA	1.97	0.46
2:C:203:ILE:HG13	2:C:204:VAL:HG23	1.96	0.46
1:A:344:HIS:HE1	1:A:376:TYR:CD2	2.33	0.46
2:C:111:LYS:O	2:C:115:GLU:HG3	2.14	0.46
1:A:184:MET:HE2	1:A:188:PHE:HB2	1.98	0.46
1:B:323:LYS:HE2	1:B:324:TYR:CE1	2.51	0.46
1:A:110:LEU:HD11	1:A:217:ILE:CD1	2.46	0.46
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.51	0.46
2:C:98:HIS:HD2	2:C:297:ASP:OD1	1.99	0.46
1:A:355:PRO:CG	1:A:403:ILE:HD13	2.43	0.46
1:A:313:TRP:CZ2	1:A:318:ILE:HD11	2.50	0.45
1:A:121:THR:HG21	1:A:140:GLN:CG	2.46	0.45
2:D:169:GLU:O	2:D:170:ALA:C	2.58	0.45
2:D:324:TRP:O	2:D:327:PRO:HD2	2.15	0.45
1:A:291:GLU:OE1	1:A:343:HIS:HE1	2.00	0.45
1:B:232:THR:HB	1:B:233:PRO:HD3	1.99	0.45
2:D:336:MET:HE2	2:D:384:VAL:HG12	1.98	0.45
3:E:40:THR:C	3:E:41:THR:HG23	2.41	0.45
1:A:30:ARG:HD3	1:A:31:TRP:NE1	2.31	0.45
1:B:313:TRP:CZ2	1:B:318:ILE:HD11	2.51	0.45
2:C:211:THR:C	2:C:214:PRO:HD2	2.41	0.45
2:D:145:ILE:O	2:D:149:TRP:HB3	2.17	0.45
1:A:171:ALA:O	1:A:175:ARG:HB3	2.18	0.44
1:A:318:ILE:HD12	1:A:318:ILE:N	2.32	0.44
1:A:114:GLU:CD	1:A:147:HIS:HB3	2.42	0.44
1:B:50:TYR:CD2	1:B:257:ILE:HD12	2.51	0.44
1:B:227:ASN:HD21	1:B:296:PHE:H	1.66	0.44
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.49	0.44
2:D:262:ARG:HA	2:D:266:GLN:HB3	2.00	0.44
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.47	0.44
7:B:3868:HOH:O	3:F:144:ASN:HB3	2.18	0.44
3:E:59:LYS:HG2	7:E:209:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:55:TRP:CZ2	3:F:59:LYS:HE2	2.53	0.44
1:B:206:LEU:HD23	1:B:271:LEU:HD13	2.00	0.44
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.53	0.44
1:B:408:PHE:CE2	1:B:415:ILE:HD11	2.53	0.44
2:D:136:MET:HE2	2:D:274:ASP:CG	2.43	0.44
3:F:23:ASN:HD22	3:F:23:ASN:N	2.14	0.44
1:B:246:HIS:CD2	1:B:246:HIS:N	2.85	0.44
2:C:33:ASN:N	2:C:33:ASN:HD22	2.15	0.44
1:A:243:GLU:O	1:A:247:MET:HG2	2.18	0.43
2:C:126:GLY:O	2:C:130:ASP:HB2	2.18	0.43
1:A:21:THR:HG22	2:C:128:SER:CB	2.48	0.43
3:F:101:ALA:HA	3:F:106:GLU:OE2	2.18	0.43
1:A:408:PHE:CE2	1:A:415:ILE:HD11	2.54	0.43
1:B:403:ILE:HD11	1:B:507:TRP:HZ3	1.82	0.43
1:B:403:ILE:HD13	1:B:515:LEU:CD1	2.49	0.43
1:A:352:ALA:CA	1:A:404:PRO:HB2	2.38	0.43
1:A:401:GLY:HA2	1:A:515:LEU:HD23	1.98	0.43
1:A:403:ILE:HG22	1:A:405:LEU:H	1.83	0.43
1:A:232:THR:HB	1:A:233:PRO:HD3	1.99	0.43
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.84	0.43
1:B:349:LEU:HD22	1:B:415:ILE:CD1	2.46	0.43
1:A:149:HIS:CE1	2:C:105:TRP:HB2	2.54	0.43
1:A:179:PRO:HB3	1:A:469:ILE:HD13	2.01	0.43
1:A:222:GLU:HA	1:A:222:GLU:OE1	2.18	0.43
1:A:401:GLY:C	1:A:515:LEU:HD22	2.43	0.43
2:D:376:ASP:O	2:D:380:ILE:HG13	2.18	0.43
2:C:42:ARG:HB2	2:C:99:ARG:HG3	2.00	0.43
3:F:24:THR:HG22	3:F:26:GLU:H	1.84	0.43
1:A:435:THR:HG21	1:A:437:ARG:NE	2.31	0.43
1:B:38:ASP:O	1:B:39:PHE:HB3	2.18	0.43
1:A:110:LEU:HD11	1:A:217:ILE:HD11	2.00	0.42
2:C:140:TRP:NE1	2:C:145:ILE:HD11	2.34	0.42
3:F:19:ILE:HG21	3:F:60:LEU:HD12	2.01	0.42
3:F:100:ALA:O	3:F:101:ALA:C	2.62	0.42
1:A:165:PRO:HG3	7:A:3853:HOH:O	2.18	0.42
1:B:114:GLU:CD	1:B:147:HIS:HB3	2.45	0.42
2:D:179:LEU:HD23	2:D:182:TRP:CE3	2.54	0.42
1:A:365:ASP:OD2	1:A:365:ASP:C	2.62	0.42
1:B:206:LEU:HD11	1:B:321:LEU:HD11	2.00	0.42
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.55	0.42
2:D:243:GLU:HB2	2:D:320:TRP:CZ2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:PRO:HG2	3:E:159:ARG:CZ	2.49	0.42
1:A:360:ARG:HG2	1:A:498:GLN:HB2	2.02	0.42
1:B:90:ASN:HD22	1:B:90:ASN:HA	1.65	0.42
2:D:63:ILE:O	2:D:64:ALA:C	2.62	0.42
1:A:40:LYS:HD2	7:A:3976:HOH:O	2.20	0.42
1:A:90:ASN:HD22	1:A:90:ASN:HA	1.59	0.42
1:A:310:TYR:CZ	1:A:336:LYS:HD2	2.54	0.42
3:E:3:LYS:HG2	3:E:9:ASN:HA	2.02	0.42
1:B:165:PRO:HG3	7:B:3836:HOH:O	2.20	0.42
1:B:344:HIS:HE1	1:B:376:TYR:CE2	2.38	0.42
2:C:270:PRO:HB3	2:D:270:PRO:CB	2.28	0.42
1:B:460:GLU:N	1:B:461:PRO:HD3	2.34	0.42
1:A:134:LYS:HD3	2:C:161:ASN:HD21	1.85	0.41
1:B:21:THR:HG22	1:B:22:SER:N	2.35	0.41
1:B:193:ILE:HD11	2:D:82:SER:HB3	2.02	0.41
1:B:360:ARG:HG2	1:B:498:GLN:HB2	2.02	0.41
2:C:266:GLN:HB2	2:C:281:ILE:HG21	2.01	0.41
3:F:151:PRO:HB2	3:F:153:GLU:OE1	2.20	0.41
1:B:334:ASP:HB2	7:B:3820:HOH:O	2.20	0.41
2:D:340:ALA:HA	2:D:389:LYS:CE	2.43	0.41
1:B:216:LEU:HD13	1:B:286:LEU:HD22	2.01	0.41
1:B:49:LYS:CE	3:F:144:ASN:HD22	2.34	0.41
1:B:230:GLU:C	1:B:233:PRO:HD2	2.45	0.41
2:C:324:TRP:C	2:C:327:PRO:HD2	2.45	0.41
2:D:357:TYR:CD2	2:D:377:ARG:NH2	2.89	0.41
3:F:55:TRP:HE3	3:F:56:ILE:HD13	1.84	0.41
3:F:95:VAL:O	3:F:99:ASN:ND2	2.53	0.41
1:A:397:ASP:HA	1:A:398:PRO:HD3	1.79	0.41
2:C:175:THR:O	2:C:179:LEU:HB2	2.21	0.41
2:D:22:LYS:HE2	7:D:525:HOH:O	2.20	0.41
3:F:23:ASN:HD22	3:F:23:ASN:C	2.28	0.41
2:C:97:LYS:CB	7:C:4079:HOH:O	2.69	0.41
1:A:65:LYS:HB3	2:C:117:TRP:CD2	2.56	0.41
1:A:466:CYS:HB2	2:C:73:THR:HA	2.02	0.41
1:B:105:VAL:O	1:B:109:PHE:HB2	2.21	0.41
1:B:397:ASP:HA	1:B:398:PRO:HD3	1.90	0.41
2:D:143:GLU:HG2	7:D:484:HOH:O	2.19	0.41
2:D:299:TYR:O	2:D:317:MET:HE1	2.21	0.41
1:A:108:ASN:HD21	1:A:175:ARG:HH21	1.69	0.40
2:D:357:TYR:CD2	2:D:381:VAL:HG21	2.55	0.40
2:D:388:LEU:O	2:D:389:LYS:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:TRP:CD1	1:B:125:TRP:C	2.99	0.40
1:A:147:HIS:CE1	7:A:4099:HOH:O	2.74	0.40
1:B:52:MET:HA	1:B:256:SER:O	2.22	0.40
1:B:192:PHE:O	1:B:200:CYS:HB3	2.21	0.40
2:C:310:SER:O	2:C:314:ARG:HG3	2.21	0.40
3:E:120:PRO:HD3	3:E:128:PHE:CG	2.57	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	508/527 (96%)	485 (96%)	21 (4%)	2 (0%)	30	21
1	B	508/527 (96%)	487 (96%)	20 (4%)	1 (0%)	43	36
2	C	386/389 (99%)	376 (97%)	8 (2%)	2 (0%)	24	16
2	D	386/389 (99%)	368 (95%)	16 (4%)	2 (0%)	24	16
3	E	164/170 (96%)	162 (99%)	2 (1%)	0	100	100
3	F	164/170 (96%)	156 (95%)	6 (4%)	2 (1%)	10	4
All	All	2116/2172 (97%)	2034 (96%)	73 (3%)	9 (0%)	30	21

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	LYS
2	D	205	PRO
1	A	94	ARG
1	A	514	ARG
2	C	64	ALA
2	D	64	ALA

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Mol	Chain	Res	Type
3	F	74	GLU
3	F	122	ILE
2	C	251	VAL

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	425/442 (96%)	414 (97%)	11 (3%)	40	33
1	B	422/442 (96%)	415 (98%)	7 (2%)	53	49
2	C	315/323 (98%)	312 (99%)	3 (1%)	68	67
2	D	312/323 (97%)	306 (98%)	6 (2%)	50	45
3	E	143/147 (97%)	142 (99%)	1 (1%)	76	76
3	F	142/147 (97%)	138 (97%)	4 (3%)	38	30
All	All	1759/1824 (96%)	1727 (98%)	32 (2%)	51	47

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	38	ASP
1	A	90	ASN
1	A	110	LEU
1	A	112	VAL
1	A	125	TRP
1	A	175	ARG
1	A	206	LEU
1	A	302	VAL
1	A	467	GLN
1	A	514	ARG
1	B	33	GLN
1	B	90	ASN
1	B	112	VAL
1	B	125	TRP

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Mol	Chain	Res	Type
1	B	222	GLU
1	B	279	GLN
1	B	311	GLU
2	C	33	ASN
2	C	122	ARG
2	C	173	ASP
2	D	4	LEU
2	D	80	ARG
2	D	153	LEU
2	D	173	ASP
2	D	205	PRO
2	D	266	GLN
3	E	44	ARG
3	F	11	THR
3	F	23	ASN
3	F	44	ARG
3	F	164	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	78	GLN
1	A	90	ASN
1	A	100	ASN
1	A	108	ASN
1	A	155	ASN
1	A	168	HIS
1	A	203	ASN
1	A	214	ASN
1	A	227	ASN
1	A	249	ASN
1	A	259	ASN
1	A	268	ASN
1	A	273	ASN
1	A	279	GLN
1	A	343	HIS
1	A	344	HIS
1	A	413	HIS
1	A	439	HIS
1	A	442	ASN
1	A	486	HIS

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Mol	Chain	Res	Type
1	B	33	GLN
1	B	59	GLN
1	B	78	GLN
1	B	90	ASN
1	B	108	ASN
1	B	129	GLN
1	B	135	ASN
1	B	168	HIS
1	B	227	ASN
1	B	249	ASN
1	B	252	GLN
1	B	259	ASN
1	B	268	ASN
1	B	273	ASN
1	B	278	GLN
1	B	279	GLN
1	B	343	HIS
1	B	344	HIS
1	B	411	ASN
1	B	413	HIS
1	B	422	GLN
1	B	439	HIS
1	B	451	GLN
1	B	472	GLN
1	B	486	HIS
1	B	527	ASN
2	C	33	ASN
2	C	98	HIS
2	C	146	ASN
2	C	161	ASN
2	C	266	GLN
2	C	282	ASN
2	C	285	GLN
2	C	301	ASN
2	C	379	GLN
2	D	98	HIS
2	D	161	ASN
2	D	285	GLN
2	D	296	GLN
2	D	301	ASN
3	E	23	ASN
3	E	34	GLN

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Mol	Chain	Res	Type
3	E	45	ASN
3	E	144	ASN
3	E	158	GLN
3	E	165	HIS
3	E	167	GLN
3	F	7	HIS
3	F	23	ASN
3	F	39	HIS
3	F	45	ASN
3	F	99	ASN
3	F	144	ASN
3	F	158	GLN
3	F	167	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	$\# Z > 2$
6	BRJ	B	3800	4	3,3,3	0.42	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BRJ	B	3809	-	3,3,3	0.43	0	2,2,2	0.21	0
6	BRJ	C	3811	-	3,3,3	0.44	0	2,2,2	0.14	0
6	BRJ	C	3808	-	3,3,3	0.44	0	2,2,2	0.21	0
6	BRJ	C	3807	-	3,3,3	0.39	0	2,2,2	0.29	0
6	BRJ	A	3803	4	3,3,3	0.41	0	2,2,2	0.21	0
6	BRJ	B	3801	-	3,3,3	0.42	0	2,2,2	0.30	0
6	BRJ	A	3805	-	3,3,3	0.58	0	2,2,2	0.47	0
6	BRJ	C	3810	-	3,3,3	0.42	0	2,2,2	0.22	0
6	BRJ	B	3802	-	3,3,3	0.37	0	2,2,2	0.42	0
6	BRJ	A	3806	-	3,3,3	0.49	0	2,2,2	0.18	0
6	BRJ	A	3804	-	3,3,3	0.39	0	2,2,2	0.26	0

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
6	BRJ	B	3800	4	-	0/1/1/1	-
6	BRJ	B	3809	-	-	0/1/1/1	-
6	BRJ	C	3811	-	-	0/1/1/1	-
6	BRJ	C	3808	-	-	0/1/1/1	-
6	BRJ	C	3807	-	-	0/1/1/1	-
6	BRJ	A	3803	4	-	0/1/1/1	-
6	BRJ	B	3801	-	-	1/1/1/1	-
6	BRJ	A	3805	-	-	1/1/1/1	-
6	BRJ	C	3810	-	-	0/1/1/1	-
6	BRJ	B	3802	-	-	1/1/1/1	-
6	BRJ	A	3806	-	-	0/1/1/1	-
6	BRJ	A	3804	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	3805	BRJ	BR1-CB-CB1-OB1
6	B	3802	BRJ	BR1-CB-CB1-OB1
6	A	3804	BRJ	BR1-CB-CB1-OB1
6	B	3801	BRJ	BR1-CB-CB1-OB1

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	3808	BRJ	1	0
6	C	3807	BRJ	1	0
6	A	3805	BRJ	1	0

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	510/527 (96%)	0.10	20 (3%) 43 50	13, 22, 43, 71	0
1	B	510/527 (96%)	0.10	15 (2%) 53 60	14, 23, 41, 73	0
2	C	388/389 (99%)	-0.26	7 (1%) 67 75	11, 18, 40, 66	0
2	D	388/389 (99%)	0.76	50 (12%) 7 9	16, 31, 55, 83	0
3	E	166/170 (97%)	-0.08	6 (3%) 46 53	12, 20, 38, 67	0
3	F	166/170 (97%)	1.75	66 (39%) 1 0	24, 42, 64, 81	0
All	All	2128/2172 (97%)	0.27	164 (7%) 19 22	11, 24, 50, 83	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	4	LEU	7.9
3	F	4	LEU	6.3
3	F	83	PHE	5.0
3	E	168	SER	4.4
2	D	352	ILE	4.3
3	F	19	ILE	4.1
3	F	23	ASN	4.0
2	D	385	LEU	3.8
3	F	71	ALA	3.8
2	D	380	ILE	3.8
3	F	80	LYS	3.7
1	A	54	ASN	3.6
3	F	16	VAL	3.6
2	D	353	THR	3.6
1	A	514	ARG	3.6
3	F	22	LEU	3.6
3	F	25	LEU	3.6
3	F	161	VAL	3.5
2	D	374	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	389	LYS	3.5
2	C	270	PRO	3.4
3	E	23	ASN	3.4
3	F	60	LEU	3.4
1	A	19	ALA	3.3
3	F	28	ALA	3.3
3	F	24	THR	3.3
2	D	350	GLU	3.2
3	F	100	ALA	3.2
2	C	131	GLY	3.2
3	E	22	LEU	3.2
3	F	5	GLY	3.2
1	B	403	ILE	3.1
3	F	67	LEU	3.1
2	D	375	ALA	3.1
1	A	310	TYR	3.1
2	D	205	PRO	3.1
3	F	32	LEU	3.0
2	D	373	PHE	3.0
3	F	70	ARG	3.0
1	B	259	ASN	3.0
1	A	515	LEU	3.0
2	D	371	ILE	3.0
1	B	320	ARG	2.9
3	F	73	ASN	2.9
2	D	377	ARG	2.9
2	D	387	GLY	2.9
3	F	20	ALA	2.9
3	F	118	TYR	2.9
3	F	122	ILE	2.9
2	D	360	VAL	2.8
2	D	354	ALA	2.8
3	F	69	ALA	2.8
2	D	384	VAL	2.8
3	F	75	VAL	2.8
1	B	442	ASN	2.7
3	F	35	PHE	2.7
1	A	18	ARG	2.7
3	F	72	PHE	2.7
1	A	318	ILE	2.7
1	A	403	ILE	2.7
1	A	20	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
3	F	91	LEU	2.6
2	D	93	VAL	2.6
3	F	93	GLY	2.6
3	E	3	LYS	2.6
3	F	84	GLY	2.6
2	C	389	LYS	2.6
3	F	77	PHE	2.6
2	D	370	ARG	2.6
2	D	365	GLU	2.6
2	D	311	ASP	2.5
1	B	527	ASN	2.5
3	F	89	SER	2.5
3	F	120	PRO	2.5
2	D	349	LYS	2.5
1	A	316	ILE	2.5
1	B	490	SER	2.5
1	A	389	GLU	2.5
2	D	347	THR	2.5
2	D	381	VAL	2.5
1	A	21	THR	2.4
3	F	14	ALA	2.4
3	F	33	LYS	2.4
1	B	77	ARG	2.4
3	F	78	ARG	2.4
2	D	135	ALA	2.4
3	F	82	ALA	2.4
3	F	26	GLU	2.4
3	F	64	VAL	2.4
3	F	164	VAL	2.4
2	C	275	ASN	2.4
2	D	348	ASP	2.4
2	D	7	ARG	2.4
3	F	65	ALA	2.4
3	F	153	GLU	2.4
3	F	160	GLY	2.4
1	A	409	ILE	2.3
1	B	54	ASN	2.3
3	F	17	ASN	2.3
1	B	317	TRP	2.3
2	D	363	TRP	2.3
1	A	435	THR	2.3
2	D	357	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
3	F	11	THR	2.3
2	D	329	ILE	2.3
2	D	376	ASP	2.3
3	F	90	VAL	2.3
3	E	153	GLU	2.3
3	F	30	GLU	2.3
3	F	97	LYS	2.3
2	D	270	PRO	2.3
2	D	368	ALA	2.3
3	F	29	ALA	2.3
2	D	206	GLY	2.3
1	A	397	ASP	2.3
3	F	74	GLU	2.3
3	F	66	VAL	2.3
3	F	79	HIS	2.3
2	D	356	LEU	2.3
2	D	333	ARG	2.2
1	B	316	ILE	2.2
1	A	516	ASN	2.2
1	A	520	LYS	2.2
2	D	308	GLU	2.2
2	D	342	LEU	2.2
2	D	372	ASP	2.2
3	F	21	GLN	2.2
3	F	110	ILE	2.2
3	F	63	LYS	2.2
2	C	271	ARG	2.2
2	D	369	SER	2.2
2	D	340	ALA	2.2
3	F	43	PHE	2.2
1	A	302	VAL	2.2
3	F	163	VAL	2.2
1	B	260	ASP	2.2
3	F	39	HIS	2.1
1	B	504	ASP	2.1
2	D	316	VAL	2.1
3	F	121	PRO	2.1
1	B	311	GLU	2.1
3	F	56	ILE	2.1
3	F	68	LYS	2.1
2	C	308	GLU	2.1
2	C	205	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	275	ASN	2.1
2	D	301	ASN	2.1
3	F	96	ALA	2.1
2	D	366	ASP	2.1
3	F	38	ASP	2.1
1	B	328	SER	2.1
3	F	162	ARG	2.1
2	D	5	GLY	2.1
1	A	317	TRP	2.1
2	D	204	VAL	2.1
3	F	15	TRP	2.1
3	F	18	LYS	2.0
2	D	137	ASN	2.0
2	D	266	GLN	2.0
1	A	510	ASP	2.0
3	F	102	LYS	2.0
1	B	516	ASN	2.0
2	D	322	GLY	2.0
2	D	271	ARG	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	BRJ	B	3802	4/4	0.48	0.38	42,42,42,42	0
6	BRJ	A	3805	4/4	0.69	0.29	50,50,50,50	0
6	BRJ	C	3808	4/4	0.69	0.36	68,68,68,68	0
6	BRJ	B	3801	4/4	0.79	0.24	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	BRJ	C	3807	4/4	0.80	0.29	58,58,58,58	0
5	CA	A	1162	1/1	0.85	0.11	39,39,39,39	0
6	BRJ	C	3811	4/4	0.89	0.20	77,77,77,77	0
5	CA	C	1112	1/1	0.92	0.09	56,56,56,56	0
6	BRJ	C	3810	4/4	0.93	0.19	56,56,56,56	0
5	CA	C	1218	1/1	0.95	0.07	42,42,42,42	0
6	BRJ	A	3806	4/4	0.97	0.12	33,33,33,33	0
6	BRJ	B	3800	4/4	0.97	0.11	43,43,43,43	0
6	BRJ	A	3804	4/4	0.97	0.12	44,44,44,44	0
6	BRJ	A	3803	4/4	0.97	0.11	42,42,42,42	0
4	FE	B	529	1/1	0.99	0.03	26,26,26,26	0
4	FE	A	529	1/1	0.99	0.02	25,25,25,25	0
5	CA	C	1111	1/1	0.99	0.08	27,27,27,27	0
6	BRJ	B	3809	4/4	0.99	0.08	36,36,36,36	0
4	FE	B	528	1/1	1.00	0.01	19,19,19,19	0
4	FE	A	528	1/1	1.00	0.02	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.