



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:33 PM UTC

PDB ID : 1XVB / pdb_00001xvb
Title : soluble methane monooxygenase hydroxylase: 6-bromohexanol soaked structure
Authors : Sazinsky, M.H.; Lippard, S.J.
Deposited on : 2004-10-27
Resolution : 1.80 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

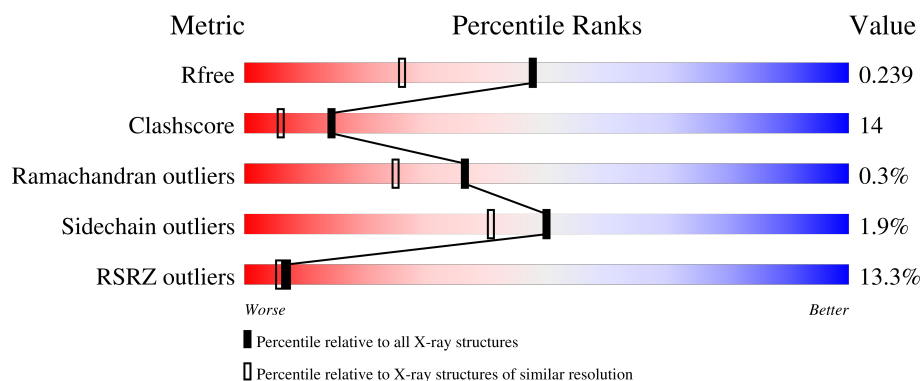
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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% 73% 22% ..
1	B	527	6% 69% 25% ..
2	C	389	2% 73% 25% .
2	D	389	31% 66% 31% .
3	E	170	7% 75% 22% ..

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Mol	Chain	Length	Quality of chain
3	F	170	52% 56% 38% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BHL	A	1210	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 18520 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
			4138	2649	709	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			

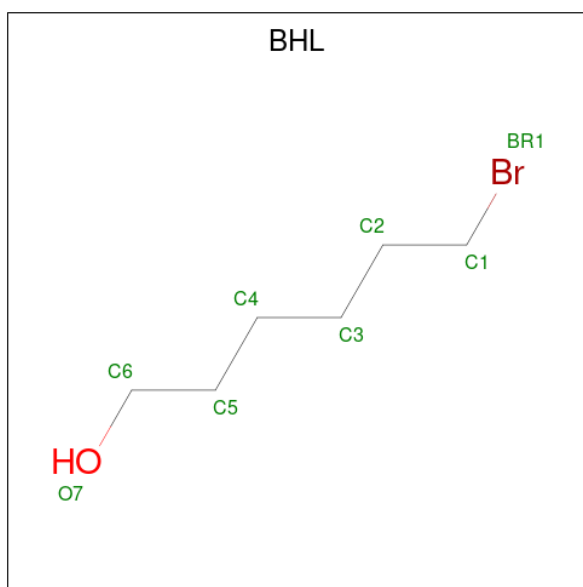
- Molecule 3 is a protein called Methane monooxygenase component A gamma chain.

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).

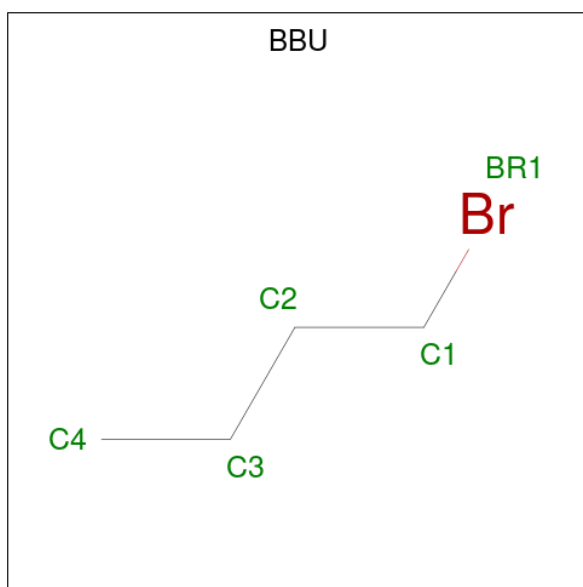
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Fe	0	0
			2	2		
4	B	2	Total	Fe	0	0
			2	2		

- Molecule 5 is 6-BROMOHEXAN-1-OL (CCD ID: BHL) (formula: C₆H₁₃BrO).



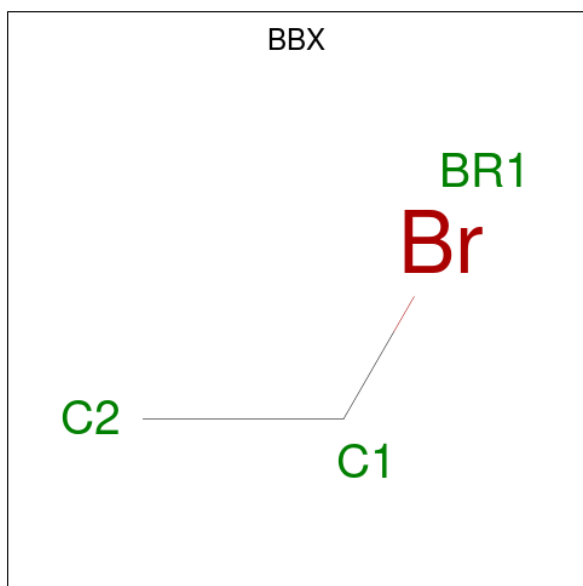
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Br	C	O	0	0
			8	1	6	1		
5	A	1	Total	Br	C	O	0	0
			8	1	6	1		
5	A	1	Total	Br	C	O	0	0
			8	1	6	1		
5	A	1	Total	Br			0	0
			1	1				
5	A	1	Total	C	O		0	0
			7	6	1			
5	B	1	Total	Br	C	O	0	0
			8	1	6	1		
5	B	1	Total	Br	C	O	0	0
			8	1	6	1		
5	B	1	Total	Br	C	O	0	0
			8	1	6	1		
5	B	1	Total	Br	C	O	0	0
			8	1	6	1		

- Molecule 6 is 1-BROMOBUTANE (CCD ID: BBU) (formula: C_4H_9Br).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Br	C	0	0
			5	1	4		

- Molecule 7 is 1-BROMOETHANE (CCD ID: BBX) (formula: C_2H_5Br).

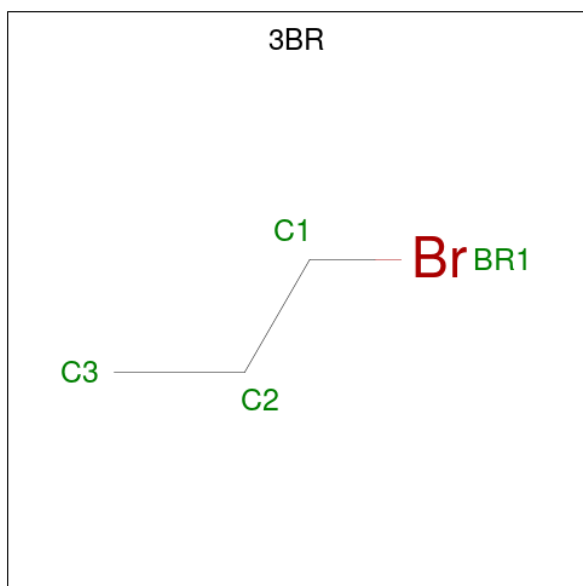


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Br	C	0	0
			3	1	2		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total Ca 1 1	0	0

- Molecule 9 is 1-BROMOPROPANE (CCD ID: 3BR) (formula: C₃H₇Br).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total Br C 4 1 3	0	0
9	C	1	Total Br C 4 1 3	0	0

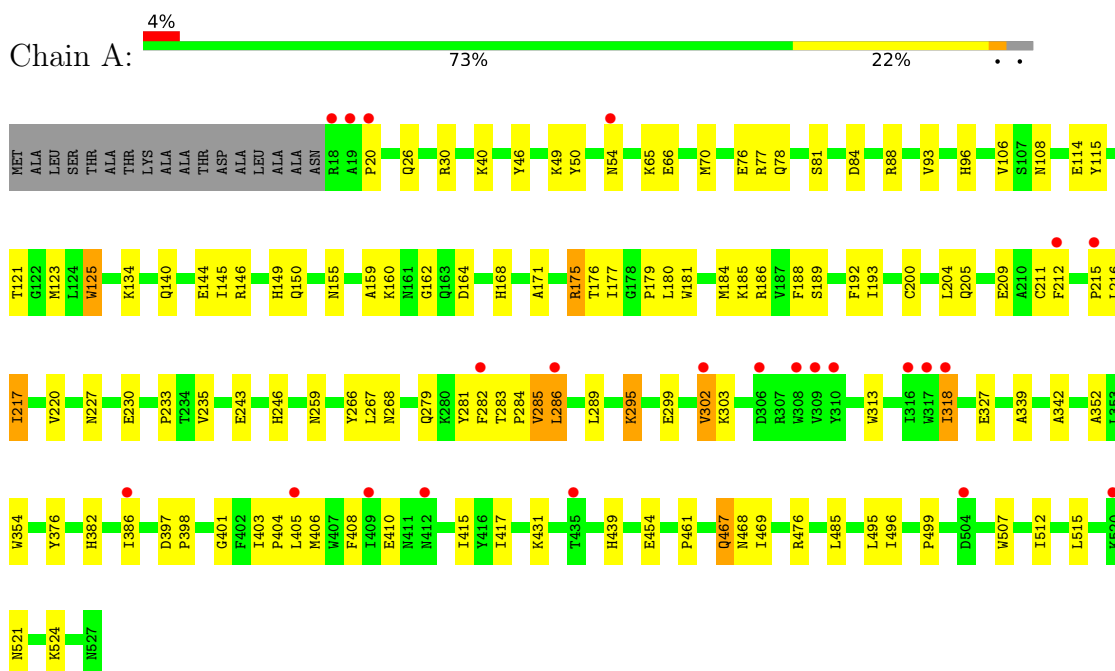
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	282	Total O 282 282	0	0
10	B	250	Total O 250 250	0	0
10	C	270	Total O 270 270	0	0
10	D	127	Total O 127 127	0	0
10	E	147	Total O 147 147	0	0
10	F	40	Total O 40 40	0	0

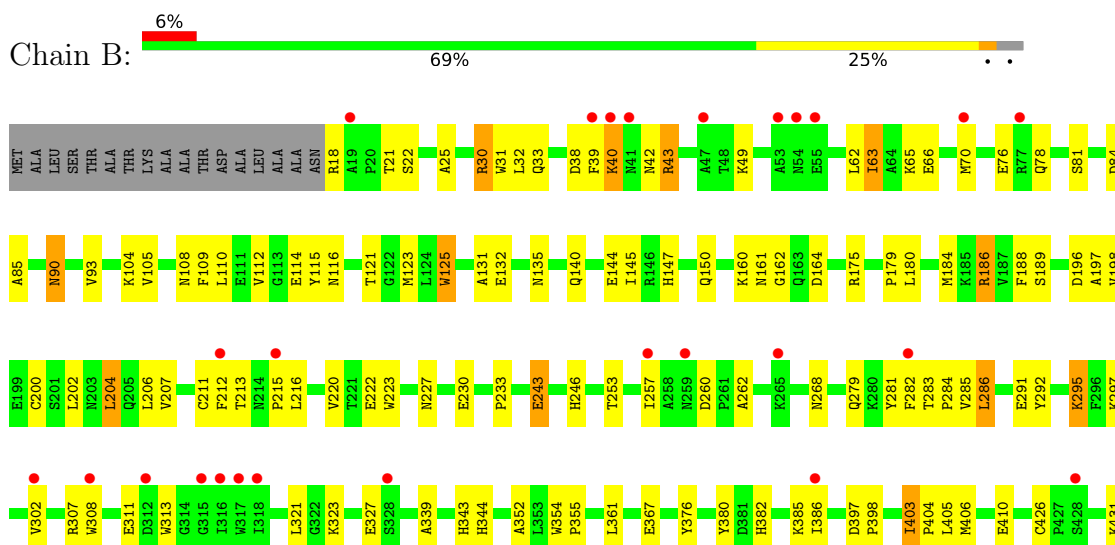
3 Residue-property plots

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: Methane monooxygenase component A alpha chain

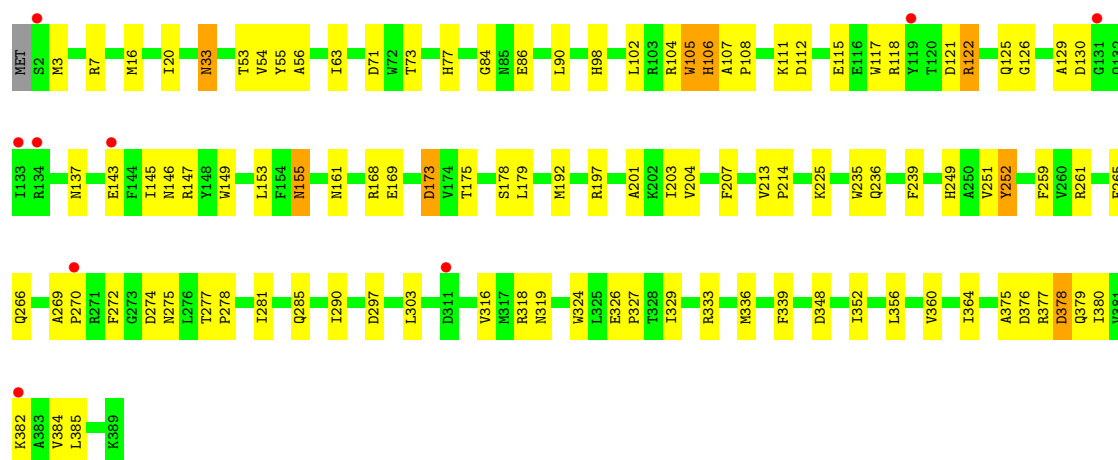
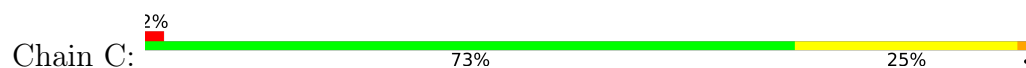


- Molecule 1: Methane monooxygenase component A alpha chain

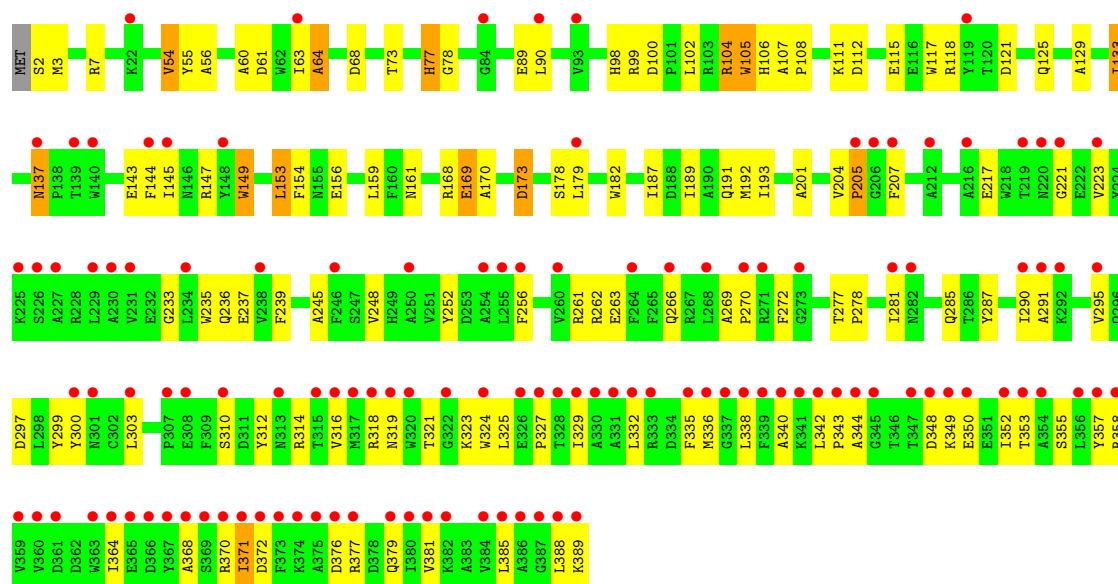




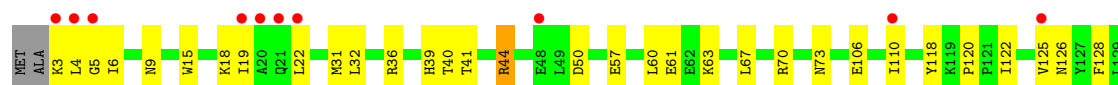
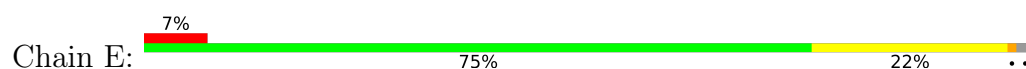
- Molecule 2: Methane monooxygenase component A beta chain



- Molecule 2: Methane monooxygenase component A beta chain

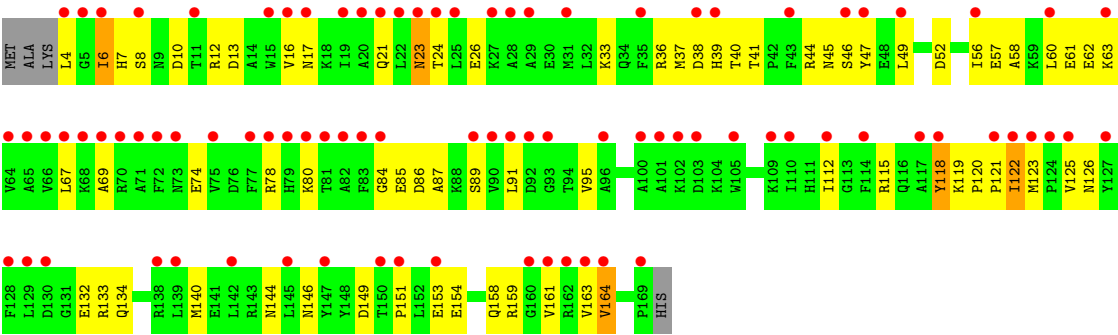


- Molecule 3: Methane monooxygenase component A gamma chain





● 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	70.63Å 171.87Å 220.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.85 – 1.80 29.85 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.1 (29.85-1.80) 91.2 (29.85-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 1.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.219 , 0.251 0.207 , 0.239	Depositor DCC
R_{free} test set	22694 reflections (9.29%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18520	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: BHL, FE, 3BR, CA, BBX, BBU

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	0.37	0/4263	0.92	18/5797 (0.3%)
1	B	0.37	0/4262	0.91	16/5796 (0.3%)
2	C	0.42	0/3259	0.89	14/4430 (0.3%)
2	D	0.34	0/3247	0.85	13/4417 (0.3%)
3	E	0.41	0/1392	0.87	4/1876 (0.2%)
3	F	0.30	0/1387	0.79	2/1873 (0.1%)
All	All	0.37	0/17810	0.89	67/24189 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	6	ILE	N-CA-C	7.88	117.83	110.42
3	E	130	ASP	N-CA-C	-7.65	102.95	111.82
1	B	496	ILE	N-CA-C	-7.60	103.38	110.53
1	B	431	LYS	N-CA-C	-7.45	104.00	113.23
1	B	339	ALA	N-CA-C	7.44	119.47	111.36
1	B	285	VAL	N-CA-C	7.44	117.52	110.53
1	A	243	GLU	N-CA-C	7.28	120.08	111.71
1	A	339	ALA	N-CA-C	6.97	118.56	110.97
2	D	204	VAL	CA-C-N	6.78	128.31	119.84
2	D	204	VAL	C-N-CA	6.78	128.31	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	106	HIS	N-CA-C	6.69	118.23	111.07
1	B	145	ILE	N-CA-C	-6.63	104.02	110.72
2	C	105	TRP	N-CA-C	-6.55	100.28	110.17
1	A	145	ILE	N-CA-C	-6.45	104.21	110.72
2	D	105	TRP	N-CA-C	-6.41	100.49	110.17
2	C	149	TRP	N-CA-C	-6.40	104.39	111.36
1	B	426	CYS	CA-C-N	6.34	125.84	119.24
1	B	426	CYS	C-N-CA	6.34	125.84	119.24
1	A	496	ILE	N-CA-C	-6.33	104.58	110.53
2	D	54	VAL	N-CA-C	6.28	117.41	108.93
1	A	164	ASP	CA-C-N	6.27	126.17	119.28
1	A	164	ASP	C-N-CA	6.27	126.17	119.28
2	C	236	GLN	N-CA-C	6.24	121.06	113.38
2	D	106	HIS	N-CA-C	6.21	118.56	111.11
1	A	431	LYS	N-CA-C	-6.13	105.62	113.23
1	A	204	LEU	N-CA-C	6.11	117.82	111.03
1	A	295	LYS	N-CA-C	-6.08	103.80	112.13
1	B	243	GLU	N-CA-C	6.00	118.61	111.71
2	C	265	PHE	N-CA-C	5.99	117.48	111.07
1	B	162	GLY	N-CA-C	5.95	121.70	112.60
1	B	295	LYS	N-CA-C	-5.90	104.05	112.13
1	A	285	VAL	N-CA-C	5.89	116.67	110.72
1	B	164	ASP	CA-C-N	5.86	125.72	119.28
1	B	164	ASP	C-N-CA	5.86	125.72	119.28
3	E	39	HIS	N-CA-C	5.82	122.34	113.61
1	A	267	LEU	N-CA-C	5.81	118.08	111.11
2	D	252	TYR	N-CA-C	5.75	117.22	111.07
2	C	56	ALA	N-CA-C	-5.73	105.04	111.28
3	F	118	TYR	N-CA-C	5.72	119.82	112.26
2	D	169	GLU	N-CA-C	5.72	120.26	113.28
3	E	118	TYR	N-CA-C	5.66	120.89	113.30
1	A	266	TYR	N-CA-C	5.65	121.60	114.31
2	D	56	ALA	N-CA-C	-5.65	105.21	111.36
3	E	73	ASN	N-CA-C	-5.63	103.26	110.53
1	A	342	ALA	N-CA-C	5.61	117.84	111.11
1	B	204	LEU	N-CA-C	5.51	118.34	111.24
1	B	403	ILE	N-CA-C	-5.50	101.06	107.61
2	C	252	TYR	N-CA-C	5.49	116.95	110.97
1	B	104	LYS	N-CA-C	-5.49	105.30	111.28
2	C	249	HIS	N-CA-C	5.48	119.13	112.23
1	A	162	GLY	N-CA-C	5.44	120.93	112.60
2	C	53	THR	N-CA-C	5.41	120.12	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	63	ILE	N-CA-C	-5.40	98.70	107.28
2	C	169	GLU	N-CA-C	5.39	120.01	113.38
1	A	193	ILE	N-CA-C	5.39	120.55	109.34
2	D	137	ASN	CA-C-N	5.37	124.83	119.24
2	D	137	ASN	C-N-CA	5.37	124.83	119.24
1	A	50	TYR	N-CA-C	5.33	117.98	110.14
2	C	77	HIS	N-CA-C	-5.30	102.20	110.10
2	C	155	ASN	N-CA-C	-5.27	105.44	111.14
2	D	149	TRP	N-CA-C	-5.27	105.45	111.14
2	D	77	HIS	N-CA-C	-5.25	102.28	110.10
2	D	104	ARG	N-CA-C	5.22	116.82	108.41
2	C	104	ARG	N-CA-C	5.14	116.69	108.41
1	A	217	ILE	N-CA-C	5.12	115.27	110.30
1	B	93	VAL	N-CA-C	5.11	116.53	111.67
1	A	205	GLN	N-CA-C	5.05	119.28	111.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	46	TYR	Sidechain

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	4138	0	3897	123	0
1	B	4137	0	3888	130	0
2	C	3163	0	2986	83	0
2	D	3151	0	2960	110	0
3	E	1364	0	1352	30	0
3	F	1358	0	1335	65	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	32	0	43	18	0
5	B	40	0	54	10	0
6	A	5	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	3	0	0	0	0
8	C	1	0	0	0	0
9	C	8	0	10	0	0
10	A	282	0	0	11	0
10	B	250	0	0	4	0
10	C	270	0	0	9	0
10	D	127	0	0	1	0
10	E	147	0	0	0	0
10	F	40	0	0	1	0
All	All	18520	0	16532	478	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 14.

All (478) 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:282:PHE:HB2	5:B:1205:BHL:O7	1.29	1.28
3:E:19:ILE:HD12	3:E:60:LEU:HD13	1.47	0.95
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.14	0.94
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.18	0.92
1:A:77:ARG:HG2	1:B:84:ASP:HB2	1.52	0.91
1:B:282:PHE:CB	5:B:1205:BHL:O7	2.20	0.89
3:F:41:THR:O	3:F:44:ARG:HD2	1.72	0.88
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.55	0.88
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.74	0.88
1:B:268:ASN:HD21	1:B:327:GLU:H	1.18	0.87
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.57	0.86
3:F:80:LYS:HE2	3:F:84:GLY:HA2	1.58	0.86
1:A:227:ASN:HD21	1:A:295:LYS:H	1.24	0.85
2:C:84:GLY:HA3	10:C:1335:HOH:O	1.74	0.85
1:B:160:LYS:HE3	1:B:161:ASN:OD1	1.79	0.83
1:A:268:ASN:HD21	1:A:327:GLU:H	1.27	0.82
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.25	0.80
3:E:15:TRP:O	3:E:19:ILE:HG12	1.82	0.79
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.64	0.78
3:E:36:ARG:HH12	3:E:122:ILE:HD13	1.49	0.77
2:C:86:GLU:HG2	10:C:1335:HOH:O	1.85	0.77
2:D:325:LEU:O	2:D:329:ILE:HG12	1.85	0.76
1:A:184:MET:HE2	1:A:188:PHE:HB2	1.68	0.76
1:A:216:LEU:HD21	5:A:1207:BHL:BR1	2.41	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:41:THR:O	3:E:44:ARG:HD2	1.85	0.76
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.68	0.75
1:B:184:MET:HE2	1:B:188:PHE:HB2	1.67	0.75
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.22	0.75
2:D:256:PHE:HA	2:D:332:LEU:HD21	1.68	0.75
1:A:467:GLN:HE22	2:C:71:ASP:H	1.35	0.74
1:B:123:MET:HE3	1:B:197:ALA:HA	1.69	0.74
2:D:371:ILE:HD13	2:D:371:ILE:H	1.51	0.74
1:A:408:PHE:HB3	5:A:1210:BHL:O7	1.87	0.73
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.70	0.73
1:B:43:ARG:HD2	1:B:43:ARG:O	1.88	0.72
1:B:30:ARG:HD3	1:B:30:ARG:C	2.14	0.72
1:A:401:GLY:HA2	1:A:515:LEU:HD21	1.70	0.72
1:A:467:GLN:H	1:A:467:GLN:HE21	1.34	0.72
1:B:268:ASN:ND2	1:B:327:GLU:H	1.88	0.72
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.72	0.71
1:A:405:LEU:CD1	5:A:1210:BHL:H41	2.21	0.71
2:D:349:LYS:HG3	2:D:352:ILE:HD11	1.72	0.71
1:A:217:ILE:HG12	5:A:1203:BHL:BR1	2.46	0.70
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.22	0.69
2:D:133:ILE:HD13	2:D:133:ILE:O	1.92	0.69
1:A:77:ARG:CG	1:B:84:ASP:HB2	2.23	0.69
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.91	0.68
3:F:13:ASP:O	3:F:16:VAL:HG22	1.94	0.68
1:A:175:ARG:HG3	1:A:181:TRP:CD2	2.29	0.68
1:B:282:PHE:HB2	5:B:1205:BHL:HO7	1.57	0.68
2:C:318:ARG:NH2	10:C:1387:HOH:O	2.27	0.68
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.40	0.68
2:D:340:ALA:HA	2:D:389:LYS:HE2	1.76	0.67
3:E:19:ILE:CD1	3:E:60:LEU:HD13	2.24	0.67
1:A:282:PHE:CE2	1:A:286:LEU:HD12	2.29	0.67
1:B:125:TRP:HE1	2:D:161:ASN:ND2	1.91	0.67
2:D:262:ARG:HA	2:D:266:GLN:HB3	1.77	0.67
1:B:33:GLN:HE22	1:B:132:GLU:H	1.40	0.66
2:D:277:THR:HG22	2:D:281:ILE:HD13	1.76	0.66
1:B:307:ARG:HH21	1:B:308:TRP:HE1	1.44	0.66
1:A:76:GLU:HG2	1:B:76:GLU:OE2	1.95	0.66
1:A:467:GLN:H	1:A:467:GLN:NE2	1.94	0.66
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.78	0.66
1:A:20:PRO:HG3	2:C:129:ALA:HB2	1.77	0.65
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:LEU:HD21	5:A:1210:BHL:C1	2.27	0.65
3:F:57:GLU:O	3:F:61:GLU:HG3	1.98	0.64
1:A:268:ASN:ND2	1:A:327:GLU:H	1.95	0.64
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.79	0.64
2:C:336:MET:HE2	2:C:384:VAL:HG12	1.77	0.64
3:E:67:LEU:HD23	3:E:70:ARG:HH21	1.62	0.64
2:C:360:VAL:O	2:C:364:ILE:HG12	1.98	0.63
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.28	0.63
3:E:165:HIS:HE1	3:E:167:GLN:NE2	1.96	0.63
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.80	0.63
1:B:282:PHE:CE2	1:B:286:LEU:HD12	2.33	0.63
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.81	0.63
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.82	0.62
1:B:367:GLU:HG3	10:B:1347:HOH:O	1.98	0.62
2:D:323:LYS:HB2	3:F:78:ARG:NH1	2.14	0.62
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.47	0.62
1:A:160:LYS:HE3	10:A:1404:HOH:O	2.00	0.62
1:B:398:PRO:HG3	1:B:507:TRP:CD1	2.34	0.62
1:A:405:LEU:HD12	5:A:1210:BHL:H41	1.80	0.62
1:B:283:THR:HB	1:B:284:PRO:HD3	1.81	0.62
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.97	0.62
1:A:114:GLU:OE1	5:A:1203:BHL:H62	2.00	0.62
1:A:405:LEU:CD1	5:A:1210:BHL:C4	2.78	0.62
1:A:467:GLN:NE2	2:C:71:ASP:H	1.97	0.62
1:B:462:GLU:HG3	3:F:112:ILE:HD11	1.82	0.62
1:A:40:LYS:HD2	10:A:1314:HOH:O	1.99	0.61
1:B:123:MET:HE1	1:B:200:CYS:SG	2.39	0.61
1:B:33:GLN:NE2	1:B:132:GLU:H	1.97	0.61
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.81	0.61
1:B:227:ASN:HD21	1:B:295:LYS:H	1.46	0.61
1:A:382:HIS:O	1:A:386:ILE:HG12	2.01	0.61
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.65	0.61
3:E:41:THR:O	3:E:44:ARG:CD	2.49	0.61
1:B:184:MET:HE3	1:B:184:MET:HA	1.82	0.60
1:B:123:MET:HB2	2:D:168:ARG:HD3	1.83	0.60
1:B:43:ARG:HD2	1:B:43:ARG:C	2.26	0.60
2:C:336:MET:CE	2:C:385:LEU:HD23	2.32	0.60
1:A:66:GLU:O	1:A:70:MET:HG2	2.02	0.60
1:B:281:TYR:O	1:B:284:PRO:HD2	2.02	0.60
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.83	0.60
2:D:223:VAL:HG13	2:D:335:PHE:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ILE:HD11	1:A:469:ILE:HG12	1.84	0.59
3:E:36:ARG:NH1	3:E:122:ILE:HD13	2.18	0.59
1:B:18:ARG:O	2:D:129:ALA:HA	2.02	0.59
2:D:153:LEU:C	2:D:153:LEU:HD12	2.27	0.59
2:C:143:GLU:HG3	10:C:1363:HOH:O	2.01	0.59
1:A:227:ASN:ND2	1:A:295:LYS:H	1.97	0.59
1:B:382:HIS:O	1:B:386:ILE:HG12	2.02	0.59
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.67	0.58
2:C:145:ILE:HD11	2:C:274:ASP:OD2	2.03	0.58
1:A:108:ASN:HD21	1:A:175:ARG:HE	1.50	0.58
2:C:329:ILE:HD11	2:C:380:ILE:HD12	1.85	0.58
1:B:216:LEU:HD21	5:B:1205:BHL:BR1	2.58	0.58
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.85	0.58
2:C:364:ILE:HD12	2:C:375:ALA:HB3	1.86	0.58
1:B:216:LEU:O	1:B:220:VAL:HG23	2.04	0.58
1:B:125:TRP:HE1	2:D:161:ASN:HD22	1.50	0.58
1:A:77:ARG:HG3	1:A:77:ARG:HH21	1.67	0.57
3:F:39:HIS:CD2	3:F:49:LEU:HD12	2.38	0.57
1:B:260:ASP:OD2	1:B:262:ALA:HB3	2.04	0.57
2:D:179:LEU:HD23	2:D:182:TRP:CE3	2.38	0.57
1:A:76:GLU:OE1	1:B:76:GLU:HG2	2.04	0.57
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.86	0.57
2:D:376:ASP:OD2	2:D:379:GLN:HG2	2.04	0.57
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.86	0.57
1:B:361:LEU:HD21	5:B:1202:BHL:H32	1.87	0.57
1:A:417:ILE:CD1	1:A:468:ASN:HB2	2.34	0.57
1:B:186:ARG:HA	2:D:73:THR:OG1	2.05	0.57
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.38	0.57
1:A:405:LEU:HD11	5:A:1210:BHL:C4	2.35	0.57
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.85	0.57
1:B:268:ASN:HD21	1:B:327:GLU:N	1.97	0.57
2:C:98:HIS:HE1	2:C:178:SER:OG	1.87	0.57
2:D:319:ASN:OD1	3:F:78:ARG:HD3	2.04	0.57
1:A:406:MET:O	1:A:410:GLU:HG3	2.04	0.56
3:F:58:ALA:O	3:F:62:GLU:HG3	2.05	0.56
1:A:81:SER:OG	1:B:84:ASP:HB3	2.04	0.56
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.96	0.56
2:C:333:ARG:HD2	10:C:1380:HOH:O	2.04	0.56
1:A:318:ILE:HD13	1:A:318:ILE:O	2.06	0.56
1:A:186:ARG:HA	2:C:73:THR:OG1	2.06	0.55
1:B:42:ASN:HD22	2:D:236:GLN:HE21	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLN:HG2	10:A:1310:HOH:O	2.07	0.55
1:B:180:LEU:HD13	5:B:1202:BHL:BR1	2.62	0.55
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.40	0.55
3:F:153:GLU:H	3:F:153:GLU:CD	2.14	0.55
1:A:184:MET:HE2	1:A:188:PHE:CG	2.42	0.55
3:E:57:GLU:O	3:E:61:GLU:HG3	2.05	0.55
1:B:302:VAL:HG12	10:B:1342:HOH:O	2.07	0.55
1:A:209:GLU:HG2	5:A:1203:BHL:H32	1.88	0.54
2:C:336:MET:HE3	2:C:385:LEU:HD23	1.89	0.54
2:D:357:TYR:CE1	2:D:381:VAL:HG11	2.42	0.54
2:D:352:ILE:HG13	2:D:353:THR:N	2.23	0.54
3:E:165:HIS:HE1	3:E:167:GLN:HE21	1.54	0.54
3:F:23:ASN:N	3:F:23:ASN:HD22	2.05	0.54
3:F:52:ASP:O	3:F:56:ILE:HG13	2.08	0.54
1:A:405:LEU:HD11	5:A:1210:BHL:H41	1.89	0.54
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.26	0.54
1:A:108:ASN:HD21	1:A:175:ARG:HH21	1.54	0.54
3:F:44:ARG:HG3	3:F:46:SER:O	2.08	0.54
1:B:461:PRO:HG2	3:F:159:ARG:CZ	2.37	0.54
2:D:102:LEU:HB2	2:D:104:ARG:HD2	1.90	0.54
3:F:36:ARG:HA	3:F:40:THR:HG23	1.90	0.54
1:B:108:ASN:HD21	1:B:175:ARG:HH21	1.54	0.54
1:A:108:ASN:ND2	1:A:175:ARG:HH21	2.05	0.53
1:A:184:MET:HE2	1:A:188:PHE:CB	2.37	0.53
1:A:302:VAL:HG13	10:A:1360:HOH:O	2.09	0.53
2:C:146:ASN:O	2:C:214:PRO:HG3	2.08	0.53
2:D:312:TYR:O	2:D:316:VAL:HG23	2.08	0.53
3:F:151:PRO:HB2	3:F:153:GLU:OE1	2.07	0.53
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.91	0.53
2:D:159:LEU:HD22	2:D:248:VAL:HG13	1.91	0.53
1:A:476:ARG:HD3	3:E:4:LEU:HG	1.91	0.53
1:A:417:ILE:HD12	1:A:468:ASN:HB2	1.90	0.53
1:B:257:ILE:C	1:B:257:ILE:HD12	2.34	0.53
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.55	0.53
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.90	0.53
1:A:121:THR:HG21	1:A:140:GLN:CG	2.39	0.53
1:B:144:GLU:OE2	1:B:144:GLU:HA	2.08	0.53
2:C:16:MET:O	2:C:20:ILE:HG12	2.09	0.53
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.89	0.53
1:A:140:GLN:O	1:A:144:GLU:HG2	2.09	0.53
1:B:476:ARG:HH12	3:F:6:ILE:HD12	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:310:SER:O	2:D:314:ARG:HG3	2.09	0.53
1:A:302:VAL:HG22	1:A:376:TYR:OH	2.09	0.53
2:C:153:LEU:C	2:C:153:LEU:HD12	2.34	0.53
3:F:6:ILE:HD12	3:F:6:ILE:N	2.24	0.53
2:C:348:ASP:O	2:C:352:ILE:HG12	2.08	0.52
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.06	0.52
1:A:123:MET:HB2	2:C:168:ARG:HD3	1.91	0.52
3:E:32:LEU:HD23	3:E:122:ILE:HD11	1.90	0.52
1:A:121:THR:HG21	1:A:140:GLN:HG2	1.92	0.52
1:A:302:VAL:HG22	1:A:376:TYR:CZ	2.45	0.52
3:E:3:LYS:HG2	3:E:9:ASN:HA	1.92	0.52
3:F:61:GLU:O	3:F:121:PRO:HG2	2.10	0.52
2:C:111:LYS:O	2:C:115:GLU:HG3	2.09	0.51
1:A:417:ILE:HD13	10:A:1227:HOH:O	2.09	0.51
1:B:521:ASN:OD1	1:B:523:VAL:HG12	2.10	0.51
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.45	0.51
2:D:352:ILE:CD1	2:D:388:LEU:HD11	2.40	0.51
1:A:184:MET:HE3	1:A:184:MET:HA	1.93	0.51
1:A:216:LEU:O	1:A:220:VAL:HG23	2.09	0.51
1:B:488:LEU:HD21	1:B:509:LEU:HD13	1.93	0.51
2:C:339:PHE:CE2	2:C:352:ILE:HD12	2.45	0.51
1:A:84:ASP:HB3	1:B:81:SER:OG	2.11	0.51
1:A:106:VAL:HG13	5:A:1207:BHL:BR1	2.67	0.51
1:B:361:LEU:CD2	5:B:1202:BHL:H32	2.42	0.50
2:D:192:MET:HA	2:D:192:MET:HE2	1.93	0.50
1:B:198:VAL:O	1:B:202:LEU:HG	2.11	0.50
2:D:300:TYR:CE1	2:D:370:ARG:HG3	2.46	0.50
1:A:179:PRO:HB3	1:A:469:ILE:HD13	1.93	0.50
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.76	0.50
1:A:405:LEU:HD21	5:A:1200:BHL:BR1	2.66	0.50
3:F:86:ASP:HB3	3:F:89:SER:OG	2.11	0.50
2:D:2:SER:HB2	10:D:494:HOH:O	2.10	0.50
3:F:91:LEU:O	3:F:95:VAL:HG23	2.12	0.50
1:B:25:ALA:CB	1:B:63:ILE:HD12	2.42	0.50
2:C:352:ILE:O	2:C:356:LEU:HD23	2.11	0.50
2:D:105:TRP:O	2:D:108:PRO:HD2	2.11	0.50
2:D:149:TRP:CE2	2:D:193:ILE:HD12	2.47	0.50
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.12	0.50
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.76	0.49
2:D:143:GLU:O	2:D:147:ARG:HB3	2.12	0.49
3:F:17:ASN:O	3:F:21:GLN:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:118:TYR:HB3	3:F:123:MET:HB2	1.93	0.49
1:A:318:ILE:HD13	1:A:318:ILE:C	2.36	0.49
1:B:140:GLN:O	1:B:144:GLU:HG2	2.12	0.49
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.47	0.49
1:B:33:GLN:HA	1:B:131:ALA:HB3	1.95	0.49
1:B:227:ASN:ND2	1:B:295:LYS:H	2.09	0.49
3:F:38:ASP:HA	3:F:45:ASN:HB2	1.95	0.49
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.48	0.49
2:D:277:THR:HB	2:D:278:PRO:HD3	1.95	0.49
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.94	0.48
1:A:415:ILE:HD12	5:A:1210:BHL:H62	1.96	0.48
1:B:184:MET:HE2	1:B:188:PHE:CB	2.41	0.48
2:C:143:GLU:O	2:C:147:ARG:HB3	2.14	0.48
3:E:106:GLU:O	3:E:110:ILE:HG12	2.12	0.48
1:B:213:THR:OG1	1:B:243:GLU:HG2	2.13	0.48
2:D:223:VAL:HG11	2:D:338:LEU:HB2	1.95	0.48
1:A:175:ARG:HG3	1:A:181:TRP:CE2	2.48	0.48
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.49	0.48
1:B:63:ILE:HD13	1:B:63:ILE:H	1.78	0.48
1:B:186:ARG:HD3	1:B:186:ARG:C	2.38	0.48
2:D:235:TRP:CD1	2:D:235:TRP:C	2.91	0.48
3:E:165:HIS:CE1	3:E:167:GLN:HE21	2.31	0.48
1:A:175:ARG:HG2	1:A:176:THR:N	2.27	0.48
2:D:187:ILE:O	2:D:191:GLN:HG3	2.13	0.48
1:A:88:ARG:NH2	10:A:1456:HOH:O	2.35	0.48
1:A:230:GLU:C	1:A:233:PRO:HD2	2.39	0.48
2:C:235:TRP:CD1	2:C:235:TRP:C	2.92	0.48
1:A:281:TYR:CZ	1:A:285:VAL:HG21	2.49	0.48
1:A:81:SER:HB3	1:B:85:ALA:HB2	1.96	0.47
1:B:307:ARG:HH21	1:B:308:TRP:NE1	2.12	0.47
3:F:125:VAL:HG23	3:F:126:ASN:N	2.28	0.47
3:E:4:LEU:HG	3:E:4:LEU:O	2.14	0.47
1:A:108:ASN:HD21	1:A:175:ARG:NE	2.12	0.47
1:A:408:PHE:CB	5:A:1210:BHL:O7	2.59	0.47
2:D:277:THR:HG22	2:D:281:ILE:CD1	2.42	0.47
2:D:381:VAL:O	2:D:385:LEU:HB2	2.14	0.47
3:F:63:LYS:NZ	3:F:67:LEU:HD21	2.28	0.47
1:B:30:ARG:HD3	1:B:30:ARG:O	2.15	0.47
2:D:291:ALA:O	2:D:295:VAL:HG23	2.15	0.47
1:B:230:GLU:C	1:B:233:PRO:HD2	2.39	0.47
1:B:323:LYS:HG2	10:B:1458:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:4:LEU:HD11	3:F:10:ASP:OD2	2.15	0.47
2:C:203:ILE:HG13	2:C:204:VAL:HG23	1.95	0.47
10:C:1350:HOH:O	3:E:125:VAL:HG22	2.13	0.47
1:A:88:ARG:NE	10:A:1456:HOH:O	2.35	0.47
1:A:171:ALA:O	1:A:175:ARG:HB3	2.15	0.47
2:C:192:MET:HE2	2:C:192:MET:HA	1.97	0.47
2:C:266:GLN:HB2	2:C:281:ILE:HG21	1.97	0.47
1:A:186:ARG:HD3	1:A:186:ARG:C	2.39	0.47
1:B:216:LEU:C	1:B:216:LEU:HD23	2.40	0.47
10:A:1388:HOH:O	3:E:6:ILE:HD13	2.15	0.46
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.97	0.46
3:E:40:THR:C	3:E:41:THR:HG23	2.39	0.46
3:F:33:LYS:O	3:F:37:MET:HG2	2.15	0.46
1:B:30:ARG:HD2	1:B:31:TRP:CE2	2.50	0.46
2:D:153:LEU:HD12	2:D:154:PHE:N	2.30	0.46
1:A:398:PRO:HG3	1:A:507:TRP:CD1	2.51	0.46
2:D:324:TRP:HA	2:D:327:PRO:HD2	1.96	0.46
3:F:44:ARG:HD3	3:F:47:TYR:CE1	2.50	0.46
3:F:154:GLU:O	3:F:158:GLN:HG3	2.15	0.46
1:A:289:LEU:HD23	5:A:1206:BHL:H42	1.98	0.46
3:E:22:LEU:HD21	3:E:31:MET:CE	2.46	0.46
1:A:246:HIS:N	1:A:246:HIS:CD2	2.83	0.46
1:B:121:THR:HG21	1:B:140:GLN:CG	2.46	0.46
1:B:186:ARG:HD3	1:B:186:ARG:O	2.15	0.46
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.46	0.46
1:A:282:PHE:HB2	5:A:1207:BHL:O7	2.16	0.46
2:C:122:ARG:HD3	10:C:1361:HOH:O	2.14	0.46
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.51	0.46
10:B:1320:HOH:O	2:D:187:ILE:HD12	2.15	0.46
3:E:138:ARG:NH2	3:E:142:LEU:HD21	2.31	0.46
1:A:146:ARG:HB2	2:C:106:HIS:CE1	2.51	0.46
1:B:21:THR:HG22	1:B:22:SER:N	2.32	0.45
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.50	0.45
2:C:239:PHE:HB2	3:E:126:ASN:HA	1.98	0.45
2:D:266:GLN:HB2	2:D:281:ILE:HG21	1.99	0.45
1:A:115:TYR:OH	2:C:173:ASP:HA	2.16	0.45
1:A:180:LEU:HD13	5:A:1206:BHL:BR1	2.71	0.45
2:C:102:LEU:HD11	2:C:290:ILE:HG12	1.97	0.45
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.99	0.45
3:E:122:ILE:N	3:E:122:ILE:HD12	2.30	0.45
1:B:438:VAL:HB	3:F:164:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:223:VAL:CG1	2:D:335:PHE:HA	2.47	0.45
1:A:160:LYS:HA	2:C:33:ASN:HB2	1.98	0.45
1:B:38:ASP:O	1:B:39:PHE:HB3	2.17	0.45
2:C:378:ASP:O	2:C:382:LYS:HG3	2.15	0.45
2:D:179:LEU:HD23	2:D:182:TRP:CZ3	2.52	0.45
3:F:4:LEU:HA	3:F:8:SER:O	2.16	0.45
1:A:93:VAL:HG11	2:D:3:MET:HG2	1.98	0.45
1:A:108:ASN:HD21	1:A:175:ARG:NH2	2.15	0.45
1:B:121:THR:HG21	1:B:140:GLN:CD	2.42	0.45
2:D:98:HIS:CD2	2:D:99:ARG:N	2.84	0.45
2:D:189:ILE:O	2:D:193:ILE:HG12	2.17	0.45
1:B:204:LEU:HD11	5:B:1201:BHL:H51	1.98	0.45
1:A:54:ASN:HB2	10:A:1467:HOH:O	2.15	0.45
1:B:222:GLU:OE1	2:D:7:ARG:HD3	2.16	0.45
1:B:466:CYS:HB2	2:D:73:THR:HA	1.99	0.45
2:C:54:VAL:O	2:C:55:TYR:HB2	2.16	0.45
1:A:77:ARG:CG	1:A:77:ARG:HH21	2.29	0.45
1:A:318:ILE:HD13	10:A:1464:HOH:O	2.16	0.45
2:D:60:ALA:HA	2:D:68:ASP:HB3	1.99	0.45
3:F:24:THR:HG22	3:F:26:GLU:HB3	1.98	0.45
1:A:78:GLN:HE21	1:A:235:VAL:HA	1.82	0.45
2:D:324:TRP:C	2:D:327:PRO:HD2	2.42	0.45
3:F:80:LYS:CE	3:F:84:GLY:HA2	2.39	0.45
1:A:212:PHE:HA	1:A:215:PRO:HG2	1.99	0.44
1:B:125:TRP:CD1	1:B:125:TRP:C	2.95	0.44
2:D:98:HIS:HD2	2:D:297:ASP:OD1	2.00	0.44
2:C:98:HIS:HD2	2:C:297:ASP:OD1	2.00	0.44
2:D:145:ILE:O	2:D:149:TRP:HB3	2.17	0.44
2:D:336:MET:HE3	2:D:388:LEU:HD21	1.99	0.44
1:B:196:ASP:HB2	3:F:140:MET:SD	2.57	0.44
2:C:33:ASN:N	2:C:33:ASN:HD22	2.13	0.44
1:A:268:ASN:HD21	1:A:327:GLU:N	2.05	0.44
1:B:476:ARG:HH12	3:F:6:ILE:CD1	2.30	0.44
2:D:98:HIS:HE1	2:D:178:SER:OG	1.99	0.44
2:D:377:ARG:O	2:D:381:VAL:HG23	2.17	0.44
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.81	0.44
3:F:56:ILE:O	3:F:60:LEU:HD13	2.18	0.44
2:C:376:ASP:HB3	2:C:379:GLN:HB2	2.00	0.44
3:E:120:PRO:HD3	3:E:128:PHE:CG	2.53	0.44
2:D:54:VAL:O	2:D:55:TYR:HB2	2.18	0.44
1:B:32:LEU:HD21	1:B:135:ASN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:LEU:CD1	5:B:1201:BHL:H51	2.48	0.44
3:F:115:ARG:O	3:F:119:LYS:HB2	2.18	0.44
1:A:125:TRP:HE1	2:C:161:ASN:HD22	1.66	0.43
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.53	0.43
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.48	0.43
2:C:275:ASN:C	2:C:278:PRO:HD2	2.43	0.43
2:D:121:ASP:O	2:D:125:GLN:HG3	2.18	0.43
2:D:348:ASP:HB2	2:D:350:GLU:OE1	2.18	0.43
1:B:405:LEU:HD22	5:B:1212:BHL:H22	2.01	0.43
2:C:175:THR:O	2:C:179:LEU:HB2	2.18	0.43
2:D:245:ALA:HB3	2:D:299:TYR:OH	2.17	0.43
2:D:353:THR:O	2:D:357:TYR:HD1	2.01	0.43
1:B:184:MET:HE2	1:B:188:PHE:CG	2.53	0.43
2:D:189:ILE:HD11	2:D:287:TYR:CD1	2.53	0.43
2:D:343:PRO:O	2:D:344:ALA:C	2.61	0.43
1:A:417:ILE:CD1	1:A:469:ILE:HG12	2.46	0.43
2:C:352:ILE:O	2:C:356:LEU:CD2	2.67	0.43
2:C:339:PHE:CZ	2:C:352:ILE:HD12	2.54	0.43
1:A:283:THR:HB	1:A:284:PRO:CD	2.48	0.43
1:B:105:VAL:O	1:B:109:PHE:HB2	2.19	0.43
2:C:33:ASN:HD22	2:C:33:ASN:H	1.66	0.43
2:D:111:LYS:O	2:D:115:GLU:HG3	2.18	0.43
2:D:144:PHE:CZ	2:D:342:LEU:HD23	2.53	0.43
1:A:159:ALA:O	2:C:33:ASN:HB2	2.18	0.43
1:B:212:PHE:HA	1:B:215:PRO:HG2	2.00	0.43
1:B:223:TRP:CZ3	1:B:297:LYS:HA	2.53	0.43
3:E:44:ARG:NH2	3:E:50:ASP:OD1	2.52	0.43
1:B:406:MET:O	1:B:410:GLU:HG3	2.18	0.43
2:D:239:PHE:HB2	3:F:126:ASN:HA	2.01	0.43
1:A:192:PHE:O	1:A:200:CYS:HB3	2.19	0.43
1:B:108:ASN:ND2	1:B:175:ARG:HH21	2.17	0.43
2:C:137:ASN:HB3	2:C:272:PHE:HB3	2.01	0.43
2:D:321:THR:O	2:D:325:LEU:HB2	2.18	0.43
2:D:368:ALA:O	2:D:371:ILE:HD13	2.19	0.43
3:F:6:ILE:HD12	3:F:6:ILE:H	1.83	0.43
1:A:299:GLU:CG	1:A:303:LYS:HD3	2.49	0.43
1:A:403:ILE:CD1	1:A:515:LEU:HD12	2.49	0.43
1:B:207:VAL:O	1:B:211:CYS:HB3	2.19	0.43
2:C:7:ARG:NH1	2:C:7:ARG:HB2	2.34	0.43
1:A:134:LYS:HD3	2:C:161:ASN:HD21	1.83	0.42
1:B:216:LEU:HG	1:B:286:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:364:ILE:CD1	2:C:375:ALA:HB3	2.48	0.42
3:F:12:ARG:O	3:F:16:VAL:HG13	2.19	0.42
1:A:417:ILE:HD13	1:A:468:ASN:HB2	2.01	0.42
2:D:352:ILE:HD12	2:D:388:LEU:HD11	2.00	0.42
1:A:283:THR:HB	1:A:284:PRO:HD3	2.01	0.42
1:A:403:ILE:HG22	1:A:405:LEU:H	1.85	0.42
2:C:126:GLY:O	2:C:130:ASP:HB2	2.19	0.42
1:B:90:ASN:OD1	2:C:3:MET:O	2.38	0.42
2:D:63:ILE:O	2:D:64:ALA:C	2.62	0.42
2:C:102:LEU:HD13	10:C:1407:HOH:O	2.19	0.42
2:D:77:HIS:CG	3:F:140:MET:HG2	2.54	0.42
2:D:137:ASN:HB3	2:D:272:PHE:HB3	2.02	0.42
2:D:144:PHE:CE2	2:D:342:LEU:HD23	2.55	0.42
2:D:314:ARG:O	2:D:318:ARG:HG3	2.20	0.42
3:F:40:THR:O	3:F:41:THR:OG1	2.31	0.42
1:A:299:GLU:OE1	1:A:303:LYS:HE2	2.20	0.42
2:C:121:ASP:O	2:C:125:GLN:HG3	2.20	0.42
2:D:78:GLY:O	3:F:112:ILE:HD13	2.20	0.42
3:F:38:ASP:HB2	3:F:39:HIS:CE1	2.54	0.42
1:B:344:HIS:HE1	1:B:376:TYR:CE2	2.38	0.42
1:B:452:TRP:O	1:B:456:MET:HG3	2.19	0.42
2:C:376:ASP:O	2:C:380:ILE:HG12	2.19	0.42
1:A:246:HIS:CE1	10:A:1309:HOH:O	2.72	0.42
1:B:49:LYS:HD3	3:F:140:MET:HB3	2.02	0.42
2:C:146:ASN:ND2	2:C:197:ARG:HH21	2.14	0.42
2:D:89:GLU:OE2	3:F:125:VAL:HG22	2.20	0.42
3:F:146:ASN:HB3	3:F:149:ASP:CG	2.45	0.42
1:B:405:LEU:HD12	1:B:406:MET:N	2.35	0.41
2:D:349:LYS:O	2:D:352:ILE:HG12	2.19	0.41
2:D:355:SER:HA	2:D:358:ARG:CZ	2.49	0.41
1:A:461:PRO:HG2	3:E:159:ARG:CZ	2.51	0.41
1:B:116:ASN:CG	1:B:189:SER:HA	2.45	0.41
1:B:459:ALA:C	1:B:461:PRO:HD3	2.45	0.41
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.56	0.41
1:B:63:ILE:HD13	1:B:66:GLU:HB3	2.00	0.41
1:B:343:HIS:H	1:B:343:HIS:CD2	2.39	0.41
2:C:259:PHE:CE1	2:C:356:LEU:HD22	2.56	0.41
2:C:324:TRP:C	2:C:327:PRO:HD2	2.45	0.41
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.20	0.41
3:F:133:ARG:NH1	3:F:134:GLN:HG3	2.35	0.41
1:A:397:ASP:HA	1:A:398:PRO:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:THR:O	1:B:257:ILE:HG13	2.21	0.41
2:C:277:THR:N	2:C:278:PRO:CD	2.84	0.41
1:B:114:GLU:CD	1:B:147:HIS:HB3	2.45	0.41
1:B:246:HIS:CD2	1:B:246:HIS:N	2.87	0.41
2:C:155:ASN:ND2	2:C:252:TYR:OH	2.53	0.41
3:F:23:ASN:N	3:F:23:ASN:ND2	2.65	0.41
2:C:225:LYS:HB3	10:C:1375:HOH:O	2.19	0.41
2:D:262:ARG:HA	2:D:266:GLN:CB	2.49	0.41
3:F:132:GLU:HG3	10:F:878:HOH:O	2.20	0.41
1:A:96:HIS:HB2	2:C:20:ILE:HD12	2.03	0.41
1:B:380:TYR:HE1	1:B:385:LYS:HZ3	1.66	0.41
1:B:397:ASP:HA	1:B:398:PRO:HD3	1.88	0.41
2:D:233:GLY:O	2:D:237:GLU:HB2	2.20	0.41
2:D:319:ASN:ND2	3:F:74:GLU:HA	2.35	0.41
1:B:477:GLU:O	1:B:480:GLU:HB2	2.19	0.41
2:C:90:LEU:HD13	2:C:303:LEU:HD13	2.03	0.41
1:A:149:HIS:CE1	2:C:105:TRP:HB2	2.56	0.41
1:A:185:LYS:O	1:A:189:SER:HB2	2.21	0.41
1:B:62:LEU:HD21	1:B:70:MET:HE1	2.02	0.41
1:B:65:LYS:HB3	2:D:117:TRP:CG	2.56	0.41
2:D:169:GLU:O	2:D:170:ALA:C	2.63	0.41
2:D:312:TYR:CD1	3:F:69:ALA:HB2	2.56	0.41
2:D:340:ALA:HA	2:D:389:LYS:CE	2.47	0.41
1:B:39:PHE:O	1:B:40:LYS:C	2.64	0.41
2:D:217:GLU:O	2:D:221:GLY:HA3	2.21	0.41
3:F:86:ASP:O	3:F:87:ALA:C	2.64	0.41
3:F:120:PRO:HA	3:F:122:ILE:N	2.36	0.41
1:A:177:ILE:HG12	1:A:485:LEU:HB2	2.02	0.40
1:B:49:LYS:HD3	3:F:144:ASN:HD22	1.85	0.40
1:B:405:LEU:HD12	1:B:405:LEU:C	2.46	0.40
2:D:314:ARG:NH1	2:D:372:ASP:OD1	2.54	0.40
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.55	0.40
2:D:277:THR:O	2:D:281:ILE:HD13	2.21	0.40
3:E:22:LEU:O	3:E:63:LYS:HE2	2.21	0.40
1:A:144:GLU:OE2	1:A:144:GLU:HA	2.21	0.40
1:A:495:LEU:HD11	1:A:512:ILE:HG13	2.04	0.40
1:B:403:ILE:HD11	1:B:515:LEU:HD12	2.02	0.40
2:D:133:ILE:HD13	2:D:133:ILE:C	2.44	0.40
3:F:40:THR:C	3:F:41:THR:HG23	2.46	0.40
3:F:85:GLU:OE1	3:F:118:TYR:HE2	2.04	0.40
1:A:521:ASN:HB3	1:A:524:LYS:HG2	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:TYR:OH	2:D:173:ASP:HA	2.21	0.40
2:C:316:VAL:O	2:C:319:ASN:HB3	2.22	0.40
3:E:15:TRP:CZ3	3:E:18:LYS:HD3	2.56	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%)	488 (96%)	20 (4%)	0	100	100
1	B	508/527 (96%)	486 (96%)	21 (4%)	1 (0%)	43	31
2	C	386/389 (99%)	374 (97%)	11 (3%)	1 (0%)	36	25
2	D	386/389 (99%)	360 (93%)	24 (6%)	2 (0%)	24	14
3	E	164/170 (96%)	161 (98%)	2 (1%)	1 (1%)	21	11
3	F	164/170 (96%)	152 (93%)	11 (7%)	1 (1%)	21	11
All	All	2116/2172 (97%)	2021 (96%)	89 (4%)	6 (0%)	36	25

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	LYS
2	D	205	PRO
3	F	122	ILE
2	D	64	ALA
3	E	5	GLY
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	423/442 (96%)	414 (98%)	9 (2%)	47	36
1	B	422/442 (96%)	411 (97%)	11 (3%)	40	28
2	C	315/323 (98%)	310 (98%)	5 (2%)	55	47
2	D	312/323 (97%)	307 (98%)	5 (2%)	55	47
3	E	143/147 (97%)	142 (99%)	1 (1%)	76	73
3	F	142/147 (97%)	140 (99%)	2 (1%)	59	52
All	All	1757/1824 (96%)	1724 (98%)	33 (2%)	50	41

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	125	TRP
1	A	175	ARG
1	A	259	ASN
1	A	279	GLN
1	A	286	LEU
1	A	302	VAL
1	A	318	ILE
1	A	467	GLN
1	B	30	ARG
1	B	43	ARG
1	B	63	ILE
1	B	90	ASN
1	B	110	LEU
1	B	112	VAL
1	B	125	TRP
1	B	186	ARG
1	B	279	GLN
1	B	286	LEU
1	B	311	GLU
2	C	33	ASN
2	C	122	ARG

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Mol	Chain	Res	Type
2	C	173	ASP
2	C	377	ARG
2	C	378	ASP
2	D	133	ILE
2	D	153	LEU
2	D	173	ASP
2	D	205	PRO
2	D	371	ILE
3	E	44	ARG
3	F	23	ASN
3	F	164	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) 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	227	ASN
1	A	249	ASN
1	A	268	ASN
1	A	273	ASN
1	A	279	GLN
1	A	413	HIS
1	A	439	HIS
1	A	442	ASN
1	A	467	GLN
1	A	472	GLN
1	A	486	HIS
1	A	516	ASN
1	B	33	GLN
1	B	42	ASN
1	B	59	GLN
1	B	78	GLN
1	B	90	ASN
1	B	108	ASN
1	B	133	GLN

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Mol	Chain	Res	Type
1	B	155	ASN
1	B	168	HIS
1	B	203	ASN
1	B	214	ASN
1	B	227	ASN
1	B	249	ASN
1	B	268	ASN
1	B	273	ASN
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	527	ASN
2	C	33	ASN
2	C	98	HIS
2	C	125	GLN
2	C	146	ASN
2	C	161	ASN
2	C	285	GLN
2	C	301	ASN
2	D	98	HIS
2	D	125	GLN
2	D	161	ASN
2	D	285	GLN
2	D	301	ASN
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	17	ASN
3	F	23	ASN
3	F	34	GLN
3	F	45	ASN
3	F	99	ASN
3	F	144	ASN
3	F	158	GLN

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 19 ligands modelled in this entry, 5 are monoatomic and 1 is modelled with single atom - leaving 13 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
9	3BR	C	1213	-	3,3,3	0.65	0	1,2,2	0.85	0
5	BHL	B	1201	4	7,7,7	0.38	0	6,6,6	0.75	0
5	BHL	B	1211	-	7,7,7	0.44	0	6,6,6	0.71	0
5	BHL	B	1212	-	7,7,7	0.38	0	6,6,6	0.76	0
5	BHL	A	1210	5	6,6,7	0.47	0	5,5,6	0.71	0
5	BHL	A	1203	4	7,7,7	0.32	0	6,6,6	0.75	0
5	BHL	B	1205	-	7,7,7	0.32	0	6,6,6	0.49	0
7	BBX	B	1204	-	2,2,2	0.68	0	1,1,1	0.59	0
9	3BR	C	1208	-	3,3,3	0.67	0	1,2,2	0.98	0
6	BBU	A	1209	-	4,4,4	0.37	0	2,3,3	0.54	0
5	BHL	B	1202	-	7,7,7	0.67	0	6,6,6	2.19	2 (33%)
5	BHL	A	1206	-	7,7,7	0.50	0	6,6,6	1.96	1 (16%)
5	BHL	A	1207	-	7,7,7	0.58	0	6,6,6	1.95	1 (16%)

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
9	3BR	C	1213	-	-	0/1/1/1	-
5	BHL	B	1201	4	-	1/5/5/5	-
5	BHL	B	1211	-	-	4/5/5/5	-
5	BHL	B	1212	-	-	4/5/5/5	-
5	BHL	A	1210	5	-	4/4/4/5	-
5	BHL	A	1203	4	-	1/5/5/5	-
5	BHL	B	1205	-	-	1/5/5/5	-
9	3BR	C	1208	-	-	0/1/1/1	-
6	BBU	A	1209	-	-	1/2/2/2	-
5	BHL	B	1202	-	-	4/5/5/5	-
5	BHL	A	1206	-	-	4/5/5/5	-
5	BHL	A	1207	-	-	2/5/5/5	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1206	BHL	C4-C3-C2	4.46	136.90	114.37
5	A	1207	BHL	BR1-C1-C2	4.33	133.45	112.48
5	B	1202	BHL	BR1-C1-C2	4.12	132.45	112.48
5	B	1202	BHL	C4-C3-C2	2.82	128.62	114.37

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1203	BHL	BR1-C1-C2-C3
5	A	1207	BHL	C1-C2-C3-C4
5	B	1201	BHL	BR1-C1-C2-C3
5	B	1211	BHL	C1-C2-C3-C4
5	B	1212	BHL	C1-C2-C3-C4
5	A	1206	BHL	BR1-C1-C2-C3
5	A	1207	BHL	BR1-C1-C2-C3
5	B	1202	BHL	BR1-C1-C2-C3
5	B	1202	BHL	C3-C4-C5-C6
5	A	1206	BHL	C3-C4-C5-C6
5	A	1210	BHL	C3-C4-C5-C6
5	B	1211	BHL	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
5	B	1212	BHL	C3-C4-C5-C6
5	B	1211	BHL	C2-C3-C4-C5
5	A	1210	BHL	C2-C3-C4-C5
5	B	1212	BHL	C2-C3-C4-C5
6	A	1209	BBU	C1-C2-C3-C4
5	A	1206	BHL	C1-C2-C3-C4
5	A	1210	BHL	C4-C5-C6-O7
5	B	1211	BHL	C4-C5-C6-O7
5	B	1212	BHL	C4-C5-C6-O7
5	A	1206	BHL	C4-C5-C6-O7
5	A	1210	BHL	C1-C2-C3-C4
5	B	1202	BHL	C4-C5-C6-O7
5	B	1202	BHL	C1-C2-C3-C4
5	B	1205	BHL	C3-C4-C5-C6

There are no ring outliers.

8 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1201	BHL	2	0
5	B	1212	BHL	1	0
5	A	1210	BHL	9	0
5	A	1203	BHL	3	0
5	B	1205	BHL	4	0
5	B	1202	BHL	3	0
5	A	1206	BHL	2	0
5	A	1207	BHL	3	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%)	0.39	23 (4%)	38 37	20, 31, 51, 76	0
1	B	510/527 (96%)	0.53	30 (5%)	28 27	22, 33, 53, 77	0
2	C	388/389 (99%)	0.08	9 (2%)	61 61	18, 26, 47, 87	0
2	D	388/389 (99%)	1.46	120 (30%)	1 1	24, 42, 71, 99	0
3	E	166/170 (97%)	0.42	12 (7%)	21 20	20, 30, 48, 64	0
3	F	166/170 (97%)	2.29	88 (53%)	0 0	36, 55, 75, 87	0
All	All	2128/2172 (97%)	0.71	282 (13%)	7 6	18, 34, 62, 99	0

All (282) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	352	ILE	6.6
2	C	2	SER	6.4
3	F	161	VAL	5.7
3	F	83	PHE	5.7
2	D	385	LEU	5.6
3	F	4	LEU	5.4
3	F	24	THR	5.3
3	E	4	LEU	5.2
2	D	375	ALA	5.0
3	F	19	ILE	4.6
3	F	82	ALA	4.5
2	D	380	ILE	4.4
2	D	356	LEU	4.4
3	F	72	PHE	4.3
1	A	54	ASN	4.3
3	F	93	GLY	4.3
1	B	257	ILE	4.2
3	E	22	LEU	4.2
3	F	56	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
3	F	29	ALA	4.2
2	D	266	GLN	4.1
2	D	320	TRP	4.1
3	F	66	VAL	4.1
2	D	22	LYS	4.1
2	D	360	VAL	4.0
3	F	127	TYR	4.0
2	D	371	ILE	4.0
1	A	405	LEU	4.0
3	F	112	ILE	4.0
2	D	229	LEU	3.9
2	D	370	ARG	3.9
1	B	282	PHE	3.9
2	D	339	PHE	3.9
3	F	118	TYR	3.9
3	F	128	PHE	3.9
3	F	25	LEU	3.9
3	F	60	LEU	3.8
2	D	347	THR	3.8
3	F	84	GLY	3.8
1	A	19	ALA	3.8
3	F	121	PRO	3.7
1	B	54	ASN	3.7
2	D	216	ALA	3.7
2	D	368	ALA	3.7
2	D	357	TYR	3.6
2	D	264	PHE	3.6
2	D	227	ALA	3.5
3	F	28	ALA	3.5
1	B	317	TRP	3.5
1	A	409	ILE	3.5
1	A	302	VAL	3.5
3	F	114	PHE	3.5
3	F	77	PHE	3.5
2	D	354	ALA	3.5
2	D	386	ALA	3.5
3	F	67	LEU	3.5
1	B	215	PRO	3.4
2	D	363	TRP	3.4
2	D	225	LYS	3.4
3	F	71	ALA	3.4
3	F	125	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
3	F	20	ALA	3.4
3	F	16	VAL	3.3
3	F	75	VAL	3.3
2	D	340	ALA	3.3
3	F	100	ALA	3.3
2	D	273	GLY	3.3
3	F	5	GLY	3.3
2	D	384	VAL	3.3
2	D	270	PRO	3.3
3	F	70	ARG	3.3
2	D	307	PRO	3.3
3	F	79	HIS	3.2
2	D	230	ALA	3.2
2	D	372	ASP	3.2
2	D	330	ALA	3.2
3	E	168	SER	3.2
3	F	122	ILE	3.2
3	E	3	LYS	3.2
3	F	80	LYS	3.2
1	B	318	ILE	3.1
2	C	119	TYR	3.1
2	D	205	PRO	3.1
2	D	343	PRO	3.1
2	D	310	SER	3.1
2	D	338	LEU	3.1
2	C	311	ASP	3.1
3	F	101	ALA	3.1
1	A	215	PRO	3.1
3	F	163	VAL	3.1
2	D	353	THR	3.1
2	D	381	VAL	3.1
2	D	373	PHE	3.1
3	F	23	ASN	3.1
1	A	318	ILE	3.0
2	D	148	TYR	3.0
3	F	105	TRP	3.0
1	A	18	ARG	3.0
1	B	328	SER	3.0
3	F	11	THR	3.0
2	D	379	GLN	3.0
2	D	374	LYS	3.0
2	D	382	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
3	F	31	MET	3.0
2	D	365	GLU	3.0
2	D	350	GLU	3.0
1	A	316	ILE	3.0
3	F	91	LEU	2.9
2	D	226	SER	2.9
2	D	359	VAL	2.9
1	B	39	PHE	2.9
1	B	212	PHE	2.9
2	D	318	ARG	2.9
2	D	367	TYR	2.9
2	D	388	LEU	2.9
1	B	441	TYR	2.9
2	D	271	ARG	2.9
2	D	268	LEU	2.9
3	F	142	LEU	2.9
3	F	81	THR	2.8
2	D	327	PRO	2.8
3	F	96	ALA	2.8
2	D	308	GLU	2.8
2	D	301	ASN	2.8
2	D	342	LEU	2.8
2	D	315	THR	2.8
3	E	21	GLN	2.8
2	D	295	VAL	2.8
3	F	164	VAL	2.8
2	D	389	LYS	2.8
1	B	312	ASP	2.8
2	D	179	LEU	2.8
3	F	145	LEU	2.8
3	F	124	PRO	2.8
2	D	119	TYR	2.8
1	B	19	ALA	2.8
3	F	69	ALA	2.8
3	E	167	GLN	2.8
2	D	303	LEU	2.8
1	A	317	TRP	2.8
1	B	40	LYS	2.7
3	F	35	PHE	2.7
2	D	292	LYS	2.7
3	F	27	LYS	2.7
3	F	63	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	345	GLY	2.7
2	D	348	ASP	2.7
2	D	361	ASP	2.7
1	B	316	ILE	2.7
2	D	326	GLU	2.7
3	F	39	HIS	2.7
3	F	15	TRP	2.7
3	F	160	GLY	2.7
2	D	332	LEU	2.7
2	D	238	VAL	2.7
2	D	322	GLY	2.6
2	D	344	ALA	2.6
3	E	20	ALA	2.6
3	F	21	GLN	2.6
3	F	43	PHE	2.6
3	F	22	LEU	2.6
3	F	6	ILE	2.6
1	B	53	ALA	2.6
3	F	117	ALA	2.6
1	B	55	GLU	2.6
3	F	151	PRO	2.6
2	D	281	ILE	2.6
2	D	206	GLY	2.6
1	A	520	LYS	2.6
2	D	139	THR	2.6
2	C	270	PRO	2.6
2	D	90	LEU	2.6
3	F	129	LEU	2.6
2	D	329	ILE	2.6
3	F	92	ASP	2.6
1	B	265	LYS	2.6
1	B	302	VAL	2.6
2	D	331	ALA	2.6
3	F	46	SER	2.6
2	D	377	ARG	2.5
3	F	162	ARG	2.5
1	A	212	PHE	2.5
2	D	317	MET	2.5
2	D	337	GLY	2.5
3	F	65	ALA	2.5
2	D	207	PHE	2.5
3	F	68	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
3	F	49	LEU	2.5
2	D	364	ILE	2.5
2	D	282	ASN	2.5
2	D	212	ALA	2.5
2	D	316	VAL	2.5
3	F	153	GLU	2.5
2	D	387	GLY	2.5
3	F	138	ARG	2.4
1	B	442	ASN	2.4
2	D	140	TRP	2.4
2	D	231	VAL	2.4
2	D	63	ILE	2.4
3	F	150	THR	2.4
2	D	324	TRP	2.4
1	B	41	ASN	2.4
2	D	349	LYS	2.4
2	D	313	ASN	2.4
2	D	319	ASN	2.4
3	F	64	VAL	2.4
3	F	38	ASP	2.3
2	D	255	LEU	2.3
2	D	300	TYR	2.3
1	A	20	PRO	2.3
1	B	445	MET	2.3
3	F	90	VAL	2.3
1	A	306	ASP	2.3
1	A	286	LEU	2.3
3	F	17	ASN	2.3
3	F	123	MET	2.3
1	B	315	GLY	2.3
3	F	89	SER	2.3
1	B	504	ASP	2.3
1	A	282	PHE	2.3
2	D	256	PHE	2.3
3	F	102	LYS	2.3
3	E	110	ILE	2.3
3	F	110	ILE	2.3
1	A	504	ASP	2.3
1	A	435	THR	2.3
2	D	219	THR	2.3
3	F	103	ASP	2.2
2	D	358	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	382	LYS	2.2
1	B	428	SER	2.2
3	E	5	GLY	2.2
2	C	133	ILE	2.2
3	F	109	LYS	2.2
2	D	260	VAL	2.2
2	D	376	ASP	2.2
2	D	369	SER	2.2
2	D	221	GLY	2.2
2	D	234	LEU	2.2
1	B	259	ASN	2.1
2	D	137	ASN	2.1
2	D	220	ASN	2.1
2	D	246	PHE	2.1
3	F	73	ASN	2.1
1	A	310	TYR	2.1
1	A	386	ILE	2.1
2	D	145	ILE	2.1
3	F	130	ASP	2.1
2	D	93	VAL	2.1
2	D	333	ARG	2.1
3	E	48	GLU	2.1
2	D	144	PHE	2.1
2	D	290	ILE	2.1
3	E	19	ILE	2.1
2	C	134	ARG	2.1
2	D	336	MET	2.1
2	D	291	ALA	2.1
1	B	386	ILE	2.1
1	B	77	ARG	2.1
3	F	78	ARG	2.1
2	D	328	THR	2.1
2	D	341	LYS	2.1
2	D	84	GLY	2.1
1	B	70	MET	2.1
1	A	308	TRP	2.1
1	A	309	VAL	2.1
1	B	308	TRP	2.1
2	D	223	VAL	2.1
3	E	125	VAL	2.1
1	B	47	ALA	2.1
2	D	250	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	254	ALA	2.1
3	F	8	SER	2.0
3	F	47	TYR	2.0
3	F	147	TYR	2.0
2	C	131	GLY	2.0
3	F	169	PRO	2.0
3	F	139	LEU	2.0
2	D	366	ASP	2.0
2	C	143	GLU	2.0
2	D	335	PHE	2.0
1	A	412	ASN	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(Å ²)	Q<0.9
5	BHL	A	1210	7/8	0.60	0.34	82,82,82,82	0
5	BHL	A	1203	8/8	0.79	0.27	61,61,61,61	0
5	BHL	A	1207	8/8	0.80	0.27	60,60,60,60	0
7	BBX	B	1204	3/3	0.81	0.27	83,83,83,83	0
9	3BR	C	1213	4/4	0.81	0.30	85,85,85,85	0
5	BHL	B	1212	8/8	0.82	0.24	63,63,63,63	0
5	BHL	B	1211	8/8	0.84	0.23	75,75,75,75	0
6	BBU	A	1209	5/5	0.85	0.27	71,71,71,71	0
5	BHL	B	1205	8/8	0.88	0.22	57,57,57,57	0
9	3BR	C	1208	4/4	0.90	0.23	61,61,61,61	0
5	BHL	B	1201	8/8	0.90	0.24	68,68,68,68	0
5	BHL	A	1200	1/8	0.94	0.18	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BHL	A	1206	8/8	0.95	0.14	47,47,47,47	0
5	BHL	B	1202	8/8	0.97	0.14	44,44,44,44	0
8	CA	C	1174	1/1	0.99	0.10	32,32,32,32	0
4	FE	B	1172	1/1	0.99	0.02	32,32,32,32	0
4	FE	B	1173	1/1	0.99	0.02	28,28,28,28	0
4	FE	A	1171	1/1	1.00	0.01	25,25,25,25	0
4	FE	A	1170	1/1	1.00	0.03	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.