



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:02 AM UTC

PDB ID : 1XU5 / pdb_00001xu5
Title : Soluble methane monooxygenase hydroxylase-phenol soaked
Authors : Sazinsky, M.H.; Lippard, S.J.
Deposited on : 2004-10-25
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

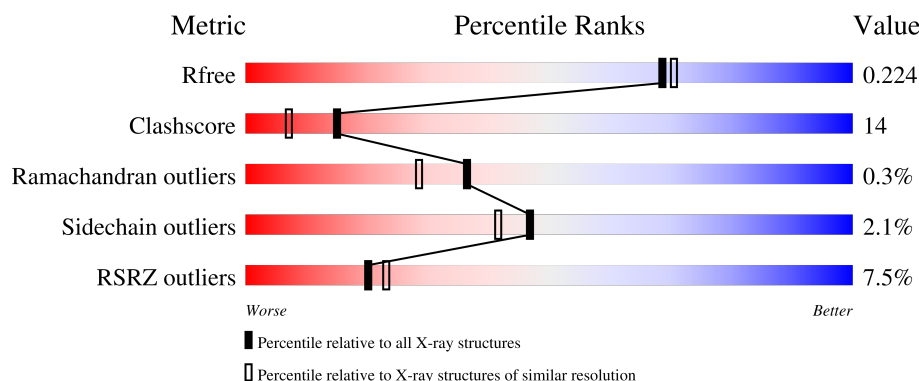
1 Overall quality at a glance

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	2% 69% 26% ..
1	B	527	4% 68% 26% ..
2	C	389	0% 78% 21% .
2	D	389	16% 68% 29% .
3	E	170	4% 75% 22% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	170	31% 69% 25%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18452 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			

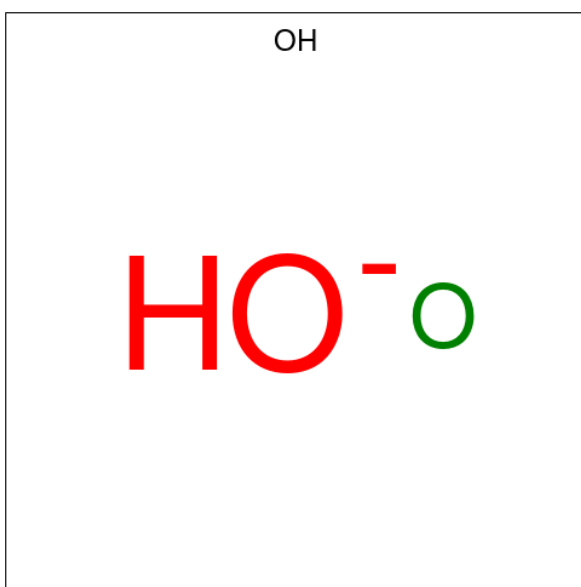
- Molecule 3 is a protein called Methane monooxygenase component A gamma chain.

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).

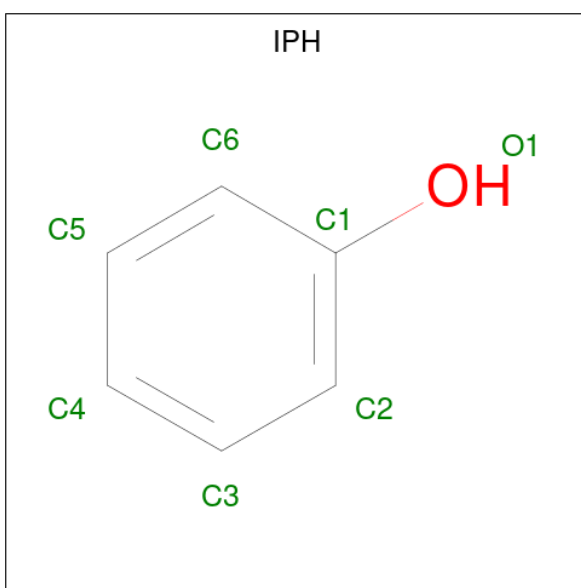
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Fe	0	0
			2	2		
4	B	2	Total	Fe	0	0
			2	2		

- Molecule 5 is HYDROXIDE ION (CCD ID: OH) (formula: HO).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	1	Total	O	0	0
			1	1		

- Molecule 6 is PHENOL (CCD ID: IPH) (formula: C₆H₆O).



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

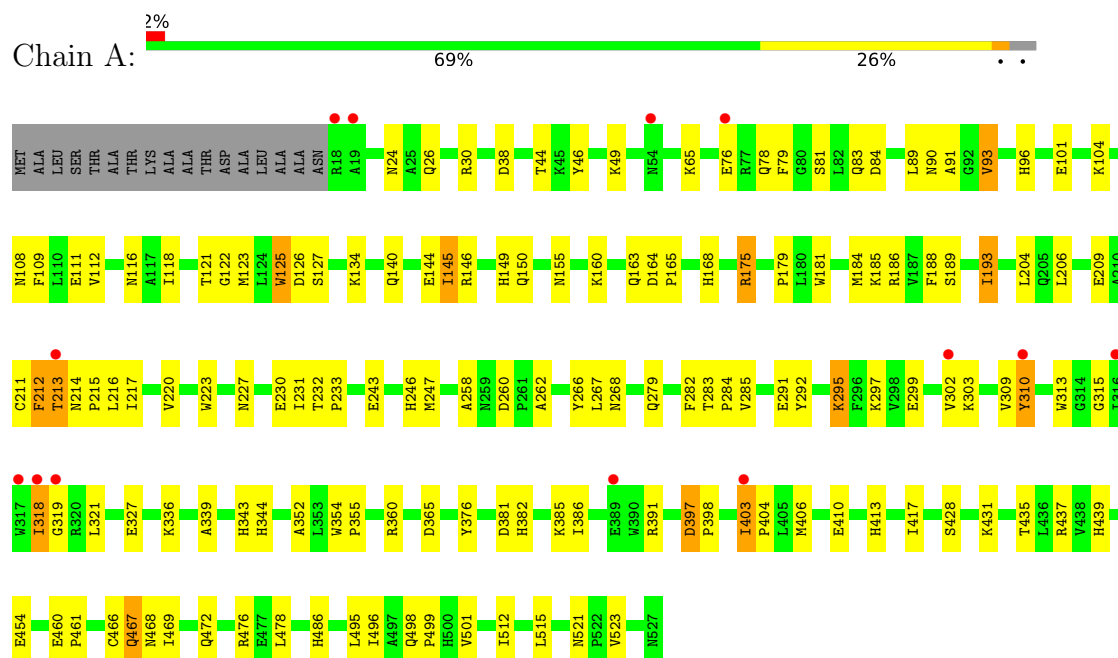
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	255	Total 255	O 255	0	0
7	B	246	Total 246	O 246	0	0
7	C	273	Total 273	O 273	0	0
7	D	159	Total 159	O 159	0	0
7	E	139	Total 139	O 139	0	0
7	F	49	Total 49	O 49	0	0

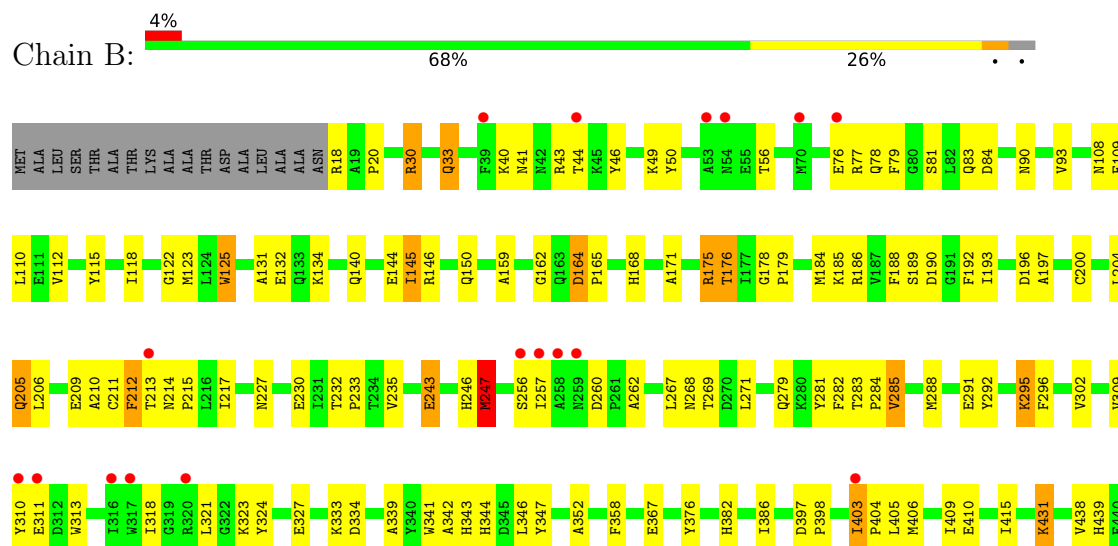
3 Residue-property plots

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.

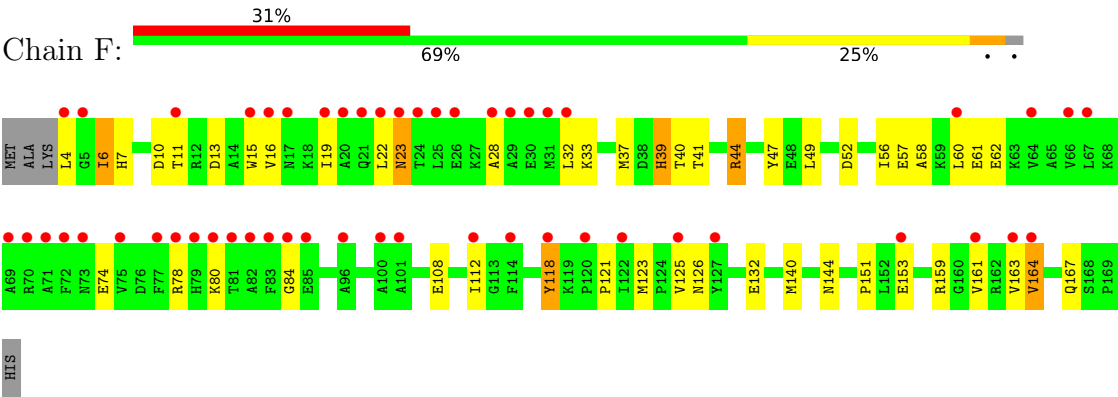
- Molecule 1: Methane monooxygenase component A alpha chain



- Molecule 1: Methane monooxygenase component A alpha chain



● Molecule 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	71.19Å 171.56Å 221.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 1.96 29.94 – 1.96	Depositor EDS
% Data completeness (in resolution range)	92.4 (29.94-1.96) 92.5 (29.94-1.96)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 1.96Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.200 , 0.228 0.197 , 0.224	Depositor DCC
R_{free} test set	8959 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.4	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	0.94	EDS
Total number of atoms	18452	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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: FE, OH, IPH

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	0.36	0/4263	0.92	21/5797 (0.4%)
1	B	0.40	0/4262	0.96	27/5796 (0.5%)
2	C	0.40	0/3259	0.89	16/4430 (0.4%)
2	D	0.34	0/3247	0.85	13/4417 (0.3%)
3	E	0.39	0/1392	0.88	6/1876 (0.3%)
3	F	0.32	0/1387	0.79	3/1873 (0.2%)
All	All	0.37	0/17810	0.90	86/24189 (0.4%)

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
2	C	0	1

There are no bond length outliers.

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	ARG	CA-C-N	9.73	135.09	120.31
1	B	175	ARG	C-N-CA	9.73	135.09	120.31
1	B	339	ALA	N-CA-C	9.63	121.54	111.14
1	B	285	VAL	N-CA-C	8.21	118.30	110.42
1	B	496	ILE	N-CA-C	-7.44	103.54	110.53
1	A	309	VAL	N-CA-C	7.43	117.51	110.53
2	C	149	TRP	N-CA-C	-7.29	103.42	111.36
1	B	431	LYS	N-CA-C	-7.24	104.26	113.23
2	D	105	TRP	N-CA-C	-7.20	99.58	109.95
1	A	266	TYR	N-CA-C	7.18	122.71	113.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	ALA	N-CA-C	7.15	118.77	110.97
2	C	106	HIS	N-CA-C	7.10	118.66	111.07
1	B	309	VAL	N-CA-C	7.06	117.17	110.53
2	C	105	TRP	N-CA-C	-6.91	99.73	110.17
1	B	243	GLU	N-CA-C	6.87	119.79	111.82
1	A	164	ASP	CA-C-N	6.78	126.38	119.19
1	A	164	ASP	C-N-CA	6.78	126.38	119.19
2	D	204	VAL	CA-C-N	6.75	128.28	119.84
2	D	204	VAL	C-N-CA	6.75	128.28	119.84
1	A	145	ILE	N-CA-C	-6.72	104.21	110.53
1	A	285	VAL	N-CA-C	6.67	116.81	110.53
1	B	164	ASP	CA-C-N	6.67	126.30	119.56
1	B	164	ASP	C-N-CA	6.67	126.30	119.56
3	E	130	ASP	N-CA-C	-6.47	104.31	111.36
3	F	39	HIS	N-CA-C	6.42	121.99	112.94
2	C	236	GLN	N-CA-C	6.31	121.14	113.38
1	A	122	GLY	N-CA-C	-6.24	104.79	112.77
3	E	122	ILE	N-CA-C	-6.18	105.12	110.74
1	B	212	PHE	N-CA-C	6.07	120.25	111.02
1	B	176	THR	CA-CB-OG1	6.04	118.66	109.60
1	A	478	LEU	N-CA-C	6.01	118.32	111.11
2	C	169	GLU	N-CA-C	5.99	120.65	113.23
1	A	267	LEU	N-CA-C	5.97	118.30	111.02
2	C	252	TYR	N-CA-C	5.93	117.44	110.97
2	D	106	HIS	N-CA-C	5.90	118.19	111.11
1	A	397	ASP	CA-C-N	5.90	125.77	119.28
1	A	397	ASP	C-N-CA	5.90	125.77	119.28
3	E	73	ASN	N-CA-C	-5.90	102.92	110.53
1	A	212	PHE	N-CA-C	5.86	120.16	112.13
1	B	342	ALA	N-CA-C	5.84	118.12	111.11
2	C	171	LEU	N-CA-C	5.84	120.03	113.02
1	B	247	MET	N-CA-C	-5.83	104.83	111.07
1	A	496	ILE	N-CA-C	-5.83	105.05	110.53
2	C	144	PHE	N-CA-C	5.82	117.70	111.36
1	B	93	VAL	N-CA-C	5.73	117.11	111.67
1	B	175	ARG	CA-C-O	-5.69	112.37	120.51
1	B	145	ILE	N-CA-C	-5.67	105.00	110.72
2	C	53	THR	N-CA-C	5.65	120.44	112.93
3	E	118	TYR	N-CA-C	5.60	120.81	113.30
3	E	39	HIS	N-CA-C	5.60	122.01	113.61
1	A	93	VAL	N-CA-C	5.60	116.62	111.81
2	D	236	GLN	N-CA-C	5.58	120.08	113.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	318	ARG	N-CA-C	-5.55	105.32	111.71
1	B	403	ILE	N-CA-C	-5.52	101.04	107.61
2	C	137	ASN	CA-C-N	5.51	124.97	119.24
2	C	137	ASN	C-N-CA	5.51	124.97	119.24
2	C	63	ILE	N-CA-C	-5.49	98.55	107.28
1	B	122	GLY	N-CA-C	-5.49	105.74	112.77
1	B	193	ILE	N-CA-C	5.48	120.73	109.34
2	D	275	ASN	N-CA-C	-5.43	106.70	113.38
2	D	252	TYR	N-CA-C	5.41	116.87	110.97
1	B	295	LYS	N-CA-C	-5.41	104.33	111.96
2	C	56	ALA	N-CA-C	-5.40	105.56	111.82
1	A	213	THR	N-CA-C	5.38	116.83	111.07
1	B	267	LEU	N-CA-C	5.38	117.56	111.11
1	A	258	ALA	N-CA-C	5.37	117.14	111.28
2	D	137	ASN	CA-C-N	5.35	125.42	119.32
2	D	137	ASN	C-N-CA	5.35	125.42	119.32
3	E	79	HIS	N-CA-C	5.32	121.51	114.12
2	D	77	HIS	N-CA-C	-5.30	102.21	110.10
1	B	178	GLY	CA-C-N	5.28	124.79	119.19
1	B	178	GLY	C-N-CA	5.28	124.79	119.19
1	B	168	HIS	N-CA-C	-5.28	105.61	111.36
1	B	162	GLY	N-CA-C	5.28	120.67	112.60
1	A	193	ILE	N-CA-C	5.26	120.27	109.34
2	D	54	VAL	N-CA-C	5.24	116.01	108.93
2	C	104	ARG	N-CA-C	5.16	116.72	108.41
1	A	104	LYS	N-CA-C	-5.15	105.56	111.07
2	C	148	TYR	N-CA-C	5.15	118.02	111.69
2	C	249	HIS	N-CA-C	5.14	118.71	112.23
1	B	205	GLN	N-CA-C	5.14	119.43	111.56
1	A	295	LYS	N-CA-C	-5.08	104.79	111.96
3	F	6	ILE	N-CA-C	5.04	119.83	109.34
3	F	118	TYR	N-CA-C	5.03	120.04	113.30
2	D	169	GLU	N-CA-C	5.01	119.66	113.50
1	A	431	LYS	N-CA-C	-5.00	107.02	113.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	299	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	124	0
1	B	4137	0	3888	141	0
2	C	3163	0	2986	67	0
2	D	3151	0	2960	106	0
3	E	1364	0	1352	33	0
3	F	1358	0	1335	46	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	7	0	6	0	0
6	B	7	0	6	0	0
7	A	255	0	0	6	0
7	B	246	0	0	6	0
7	C	273	0	0	3	0
7	D	159	0	0	4	0
7	E	139	0	0	0	0
7	F	49	0	0	4	0
All	All	18452	0	16430	461	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 (461) 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)
3:E:19:ILE:HD12	3:E:60:LEU:HD13	1.40	1.04
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.46	0.95
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.05	0.93
1:A:118:ILE:HD13	1:A:145:ILE:HD13	1.49	0.93
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.04	0.93
1:B:118:ILE:HD13	1:B:145:ILE:HD13	1.49	0.91
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.18	0.90
1:B:217:ILE:HD12	7:B:2911:HOH:O	1.74	0.87
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.25	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:GLN:HG3	7:A:2800:HOH:O	1.78	0.83
1:B:44:THR:HG22	1:B:46:TYR:H	1.42	0.83
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.43	0.83
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.61	0.81
3:E:41:THR:O	3:E:44:ARG:HD2	1.79	0.81
3:E:15:TRP:O	3:E:19:ILE:HG12	1.80	0.81
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.61	0.81
1:B:288:MET:HE1	1:B:346:LEU:CG	2.11	0.81
3:F:80:LYS:HE2	3:F:84:GLY:HA2	1.63	0.81
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.63	0.81
1:B:123:MET:HE3	1:B:197:ALA:HA	1.62	0.80
3:F:41:THR:O	3:F:44:ARG:HD2	1.80	0.80
1:A:44:THR:HG22	1:A:46:TYR:H	1.47	0.78
2:D:352:ILE:HD12	2:D:353:THR:N	2.00	0.77
1:B:268:ASN:HD21	1:B:327:GLU:H	1.33	0.77
2:C:42:ARG:HB2	2:C:99:ARG:HH11	1.48	0.77
1:B:210:ALA:HA	1:B:247:MET:HE1	1.68	0.76
1:B:288:MET:HE1	1:B:346:LEU:CB	2.16	0.75
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.84	0.75
1:A:355:PRO:HG2	1:A:403:ILE:HD13	1.67	0.75
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.68	0.75
1:A:227:ASN:HD21	1:A:295:LYS:H	1.35	0.75
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.87	0.75
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.32	0.75
1:B:403:ILE:HD12	1:B:404:PRO:HD2	1.69	0.75
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.69	0.74
1:B:382:HIS:O	1:B:386:ILE:HG12	1.88	0.74
2:D:371:ILE:HD13	2:D:371:ILE:H	1.53	0.74
3:E:19:ILE:CD1	3:E:60:LEU:HD13	2.17	0.73
1:B:209:GLU:HA	1:B:213:THR:OG1	1.88	0.73
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.19	0.73
3:E:22:LEU:HD11	3:E:31:MET:SD	2.28	0.73
2:C:3:MET:HG3	2:C:4:LEU:H	1.52	0.72
1:B:171:ALA:O	1:B:175:ARG:HG2	1.89	0.72
3:F:153:GLU:H	3:F:153:GLU:CD	1.97	0.72
1:B:288:MET:HE1	1:B:346:LEU:HG	1.71	0.72
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.85	0.72
1:A:268:ASN:HD21	1:A:327:GLU:H	1.36	0.71
3:E:98:MET:HE1	3:E:107:ALA:CB	2.20	0.71
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.56	0.71
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.20	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ILE:CD1	1:A:145:ILE:HD13	2.21	0.70
1:B:283:THR:HB	1:B:284:PRO:HD3	1.73	0.70
2:C:336:MET:CE	2:C:385:LEU:HD23	2.21	0.70
1:A:24:ASN:OD1	1:A:26:GLN:HG2	1.91	0.69
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.56	0.69
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.22	0.69
1:B:217:ILE:CD1	7:B:2911:HOH:O	2.37	0.69
2:D:167:ALA:O	2:D:176:ARG:NH1	2.25	0.69
1:B:288:MET:HE1	1:B:346:LEU:HB3	1.75	0.69
1:B:227:ASN:HD21	1:B:295:LYS:H	1.41	0.68
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.74	0.68
2:C:42:ARG:HB2	2:C:99:ARG:NH1	2.08	0.68
3:E:98:MET:HE1	3:E:107:ALA:HB2	1.76	0.68
2:C:336:MET:HE3	2:C:388:LEU:HG	1.76	0.67
3:F:4:LEU:HD11	3:F:10:ASP:OD2	1.93	0.67
1:A:175:ARG:NH1	7:A:2802:HOH:O	2.10	0.67
2:C:333:ARG:HD2	7:C:552:HOH:O	1.94	0.67
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.94	0.67
3:F:13:ASP:O	3:F:16:VAL:HG22	1.94	0.67
3:E:98:MET:HE3	3:E:98:MET:O	1.95	0.66
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.78	0.66
1:A:96:HIS:HB2	2:C:20:ILE:HD12	1.78	0.66
1:B:33:GLN:HE22	1:B:132:GLU:H	1.42	0.66
1:B:210:ALA:CA	1:B:247:MET:HE1	2.25	0.66
1:B:33:GLN:NE2	1:B:132:GLU:H	1.93	0.65
3:F:58:ALA:O	3:F:62:GLU:HG3	1.97	0.65
1:A:417:ILE:CD1	1:A:468:ASN:HB2	2.26	0.64
1:B:288:MET:HE2	1:B:347:TYR:N	2.12	0.64
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.44	0.64
1:A:76:GLU:HG2	1:B:76:GLU:OE2	1.97	0.64
1:A:175:ARG:HG3	1:A:181:TRP:CD2	2.33	0.64
1:A:382:HIS:O	1:A:386:ILE:HG12	1.97	0.64
1:B:288:MET:CE	1:B:346:LEU:HB3	2.27	0.64
3:F:52:ASP:O	3:F:56:ILE:HG12	1.98	0.64
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.61	0.64
2:D:189:ILE:O	2:D:193:ILE:HD13	1.98	0.64
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.79	0.64
2:D:325:LEU:O	2:D:329:ILE:HG12	1.98	0.63
1:A:435:THR:CG2	1:A:437:ARG:HE	2.10	0.63
1:B:123:MET:HE1	1:B:200:CYS:SG	2.39	0.63
1:B:125:TRP:HE1	2:D:161:ASN:ND2	1.97	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:LEU:O	1:B:409:ILE:HD13	1.98	0.63
2:C:3:MET:HG3	2:C:4:LEU:HD13	1.80	0.63
1:B:367:GLU:HG3	7:B:2716:HOH:O	1.99	0.63
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.80	0.63
1:B:212:PHE:O	1:B:215:PRO:HD2	1.99	0.62
1:A:417:ILE:HD13	1:A:468:ASN:HB2	1.81	0.62
1:A:160:LYS:HE3	7:A:2854:HOH:O	1.98	0.62
1:A:268:ASN:ND2	1:A:327:GLU:H	1.98	0.62
1:A:352:ALA:CA	1:A:404:PRO:HB2	2.26	0.62
1:A:118:ILE:HD13	1:A:145:ILE:CD1	2.24	0.61
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.83	0.61
2:D:153:LEU:C	2:D:153:LEU:HD12	2.25	0.61
1:B:489:ARG:HD2	1:B:495:LEU:O	2.00	0.61
1:B:108:ASN:ND2	1:B:175:ARG:HD3	2.13	0.61
1:B:281:TYR:O	1:B:284:PRO:HD2	2.00	0.61
2:C:3:MET:HG3	2:C:4:LEU:N	2.15	0.61
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.82	0.61
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.34	0.61
2:D:324:TRP:C	2:D:327:PRO:HD2	2.26	0.61
1:A:227:ASN:ND2	1:A:295:LYS:H	1.98	0.60
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.84	0.60
1:B:49:LYS:HD3	3:F:144:ASN:HD22	1.67	0.60
2:D:348:ASP:OD2	2:D:350:GLU:HB2	2.01	0.60
3:E:24:THR:HG22	3:E:27:LYS:H	1.65	0.60
2:C:3:MET:CG	2:C:4:LEU:H	2.13	0.60
1:A:155:ASN:HD22	1:A:168:HIS:CD2	2.09	0.60
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.83	0.60
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.84	0.59
3:E:98:MET:HE2	3:E:138:ARG:CG	2.32	0.59
1:A:406:MET:O	1:A:410:GLU:HG3	2.02	0.59
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.83	0.59
1:B:333:LYS:HG3	7:B:2868:HOH:O	2.02	0.59
3:F:151:PRO:HB2	3:F:153:GLU:OE1	2.02	0.58
1:A:83:GLN:HB3	1:B:77:ARG:HH12	1.67	0.58
2:D:192:MET:HE3	2:D:280:PHE:CD2	2.38	0.58
1:B:445:MET:HE3	1:B:523:VAL:HG22	1.84	0.58
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.38	0.58
1:A:495:LEU:HD11	1:A:512:ILE:HD13	1.85	0.58
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.85	0.58
1:A:213:THR:O	1:A:217:ILE:HG12	2.04	0.58
2:D:371:ILE:HD12	7:D:492:HOH:O	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.39	0.57
1:B:257:ILE:C	1:B:257:ILE:HD12	2.29	0.57
1:B:403:ILE:HD12	1:B:404:PRO:CD	2.33	0.57
3:F:19:ILE:HD12	3:F:19:ILE:C	2.28	0.57
1:A:184:MET:HE2	1:A:188:PHE:HB2	1.86	0.57
1:B:243:GLU:O	1:B:247:MET:HG2	2.05	0.57
3:F:61:GLU:O	3:F:121:PRO:HG2	2.04	0.57
1:B:406:MET:O	1:B:410:GLU:HG3	2.04	0.57
1:A:231:ILE:HD12	1:A:231:ILE:N	2.20	0.57
1:B:398:PRO:HG3	1:B:507:TRP:CD1	2.40	0.57
1:B:118:ILE:HD13	1:B:145:ILE:CD1	2.28	0.57
1:A:318:ILE:C	1:A:318:ILE:HD13	2.29	0.57
2:D:76:PHE:HZ	2:D:168:ARG:HH12	1.52	0.56
3:E:165:HIS:CE1	3:E:167:GLN:HE21	2.22	0.56
1:A:243:GLU:O	1:A:247:MET:HG2	2.05	0.56
1:A:403:ILE:HD12	1:A:515:LEU:HD13	1.88	0.56
1:A:140:GLN:O	1:A:144:GLU:HG2	2.06	0.56
1:B:164:ASP:CG	1:B:489:ARG:HH22	2.14	0.56
1:B:210:ALA:N	1:B:247:MET:HE1	2.20	0.56
1:B:227:ASN:ND2	1:B:295:LYS:H	2.02	0.56
2:C:192:MET:HE2	2:C:283:GLN:OE1	2.05	0.56
2:C:339:PHE:CE2	2:C:352:ILE:HD12	2.41	0.56
2:C:348:ASP:O	2:C:352:ILE:HG12	2.05	0.56
2:D:277:THR:HG22	2:D:281:ILE:HD13	1.88	0.56
3:E:41:THR:O	3:E:44:ARG:CD	2.53	0.56
1:A:302:VAL:HG13	1:A:376:TYR:CE2	2.40	0.55
1:B:462:GLU:HG3	3:F:112:ILE:HD11	1.86	0.55
2:D:263:GLU:HB3	2:D:355:SER:HB2	1.88	0.55
1:B:20:PRO:HB2	2:D:125:GLN:HE21	1.71	0.55
1:B:192:PHE:O	1:B:200:CYS:HB3	2.07	0.55
1:B:118:ILE:CD1	1:B:145:ILE:HD13	2.29	0.55
2:D:277:THR:HB	2:D:278:PRO:HD3	1.89	0.55
2:D:332:LEU:O	2:D:336:MET:HG2	2.06	0.55
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.72	0.55
3:E:165:HIS:HE1	3:E:167:GLN:HE21	1.54	0.55
1:B:184:MET:HE3	1:B:184:MET:HA	1.89	0.55
1:B:269:THR:HG21	7:F:188:HOH:O	2.06	0.55
3:F:57:GLU:O	3:F:61:GLU:HG3	2.07	0.55
1:A:318:ILE:HD13	1:A:318:ILE:O	2.06	0.54
2:D:352:ILE:HD12	2:D:352:ILE:C	2.31	0.54
1:B:125:TRP:HE1	2:D:161:ASN:HD22	1.56	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.25	0.54
1:A:179:PRO:HB3	1:A:469:ILE:HD13	1.88	0.54
2:D:187:ILE:O	2:D:191:GLN:HG3	2.07	0.54
1:B:108:ASN:HD21	1:B:175:ARG:HH21	1.55	0.54
1:B:184:MET:HE2	1:B:188:PHE:CG	2.42	0.54
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.38	0.54
3:E:138:ARG:NH2	3:E:142:LEU:HD21	2.23	0.54
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.73	0.54
1:A:486:HIS:HD2	7:A:2805:HOH:O	1.90	0.54
1:A:96:HIS:HB2	2:C:20:ILE:CD1	2.38	0.54
1:A:134:LYS:HD3	2:C:161:ASN:HD21	1.73	0.54
2:D:192:MET:HE2	2:D:283:GLN:OE1	2.07	0.54
3:E:165:HIS:HE1	3:E:167:GLN:NE2	2.06	0.53
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.43	0.53
1:B:403:ILE:HG23	1:B:406:MET:HG3	1.89	0.53
3:E:4:LEU:O	3:E:4:LEU:HG	2.08	0.53
1:A:355:PRO:HG2	1:A:403:ILE:CD1	2.36	0.53
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.41	0.53
1:A:435:THR:HG21	1:A:437:ARG:HE	1.73	0.53
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.90	0.53
3:E:57:GLU:O	3:E:61:GLU:HG3	2.09	0.53
2:C:175:THR:O	2:C:179:LEU:HD13	2.08	0.53
2:C:261:ARG:HE	2:C:285:GLN:NE2	2.01	0.53
1:B:438:VAL:HB	3:F:164:VAL:HG22	1.90	0.52
2:D:111:LYS:O	2:D:115:GLU:HG3	2.09	0.52
2:D:145:ILE:O	2:D:149:TRP:HB3	2.09	0.52
1:B:184:MET:HE2	1:B:188:PHE:HB2	1.92	0.52
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.45	0.52
1:B:490:SER:OG	2:D:32:ASN:HB2	2.09	0.52
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.90	0.52
3:F:80:LYS:HE2	3:F:84:GLY:CA	2.38	0.52
1:A:123:MET:HB2	2:C:168:ARG:HD3	1.91	0.52
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.42	0.52
1:B:439:HIS:HE1	1:B:454:GLU:OE1	1.93	0.52
2:C:3:MET:SD	2:D:26:GLU:O	2.67	0.52
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.07	0.52
1:A:476:ARG:HD3	3:E:4:LEU:HG	1.92	0.52
2:C:146:ASN:ND2	2:C:197:ARG:HH21	2.08	0.52
2:D:102:LEU:HB2	2:D:104:ARG:HD2	1.92	0.52
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.93	0.52
2:C:153:LEU:C	2:C:153:LEU:HD12	2.35	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:15:TRP:O	3:F:19:ILE:HG23	2.10	0.51
1:A:260:ASP:OD2	1:A:262:ALA:HB3	2.10	0.51
2:D:247:SER:O	2:D:251:VAL:HB	2.10	0.51
2:D:137:ASN:HB3	2:D:272:PHE:HB3	1.91	0.51
1:B:33:GLN:HA	1:B:131:ALA:HB3	1.93	0.51
2:C:211:THR:C	2:C:214:PRO:HD2	2.36	0.51
3:F:33:LYS:O	3:F:37:MET:HG2	2.11	0.51
1:B:30:ARG:HD3	1:B:30:ARG:C	2.36	0.51
1:B:176:THR:HG22	2:D:68:ASP:CG	2.35	0.51
1:A:101:GLU:CD	1:A:360:ARG:HD3	2.36	0.51
1:A:91:ALA:C	1:A:231:ILE:HD11	2.36	0.51
1:A:84:ASP:HB3	1:B:81:SER:OG	2.12	0.50
1:A:344:HIS:HE1	1:A:376:TYR:CD2	2.30	0.50
1:B:415:ILE:HD12	1:B:415:ILE:N	2.26	0.50
3:E:19:ILE:HD12	3:E:60:LEU:CD1	2.27	0.50
1:A:185:LYS:O	1:A:189:SER:HB2	2.11	0.50
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.46	0.50
2:D:239:PHE:HB2	3:F:126:ASN:HA	1.94	0.50
3:E:97:LYS:HE3	3:E:110:ILE:HD12	1.93	0.50
1:B:206:LEU:HD23	1:B:271:LEU:HD13	1.92	0.50
2:C:3:MET:CE	2:C:4:LEU:HD13	2.42	0.50
1:A:44:THR:HG23	1:A:126:ASP:OD1	2.12	0.50
1:B:56:THR:HG21	1:B:256:SER:OG	2.10	0.50
3:E:3:LYS:HG2	3:E:9:ASN:HA	1.94	0.50
3:F:132:GLU:HG3	7:F:194:HOH:O	2.10	0.50
1:A:193:ILE:HD11	2:C:82:SER:HB3	1.93	0.50
2:C:211:THR:O	2:C:214:PRO:HD2	2.12	0.50
2:C:235:TRP:CD1	2:C:235:TRP:C	2.90	0.49
1:A:232:THR:HB	1:A:233:PRO:HD3	1.93	0.49
2:D:324:TRP:O	2:D:327:PRO:HD2	2.12	0.49
1:B:206:LEU:HD11	1:B:321:LEU:CD1	2.42	0.49
2:C:111:LYS:O	2:C:115:GLU:HG3	2.12	0.49
2:D:98:HIS:CD2	2:D:99:ARG:N	2.80	0.49
2:D:102:LEU:HD13	2:D:290:ILE:HG23	1.93	0.49
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.95	0.49
2:D:368:ALA:O	2:D:371:ILE:HD13	2.12	0.49
3:E:58:ALA:O	3:E:62:GLU:HG3	2.13	0.49
2:D:170:ALA:O	2:D:176:ARG:NH2	2.46	0.49
2:D:261:ARG:HE	2:D:285:GLN:NE2	2.06	0.49
1:A:279:GLN:HG2	1:A:283:THR:OG1	2.13	0.49
2:D:266:GLN:HB2	2:D:281:ILE:HG21	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ARG:HA	2:C:73:THR:OG1	2.13	0.49
2:D:78:GLY:O	3:F:112:ILE:HD13	2.12	0.49
2:D:235:TRP:CD1	2:D:235:TRP:C	2.91	0.49
1:B:230:GLU:C	1:B:233:PRO:HD2	2.38	0.48
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.95	0.48
1:A:223:TRP:CZ3	1:A:297:LYS:HA	2.48	0.48
1:B:227:ASN:HD21	1:B:296:PHE:H	1.61	0.48
2:C:98:HIS:HE1	2:C:178:SER:OG	1.96	0.48
7:C:547:HOH:O	3:E:125:VAL:HG22	2.13	0.48
2:D:256:PHE:HA	2:D:332:LEU:HD21	1.95	0.48
7:D:506:HOH:O	3:F:125:VAL:HG22	2.13	0.48
1:B:140:GLN:O	1:B:144:GLU:HG2	2.14	0.48
1:B:302:VAL:CG1	1:B:376:TYR:HE2	2.24	0.48
1:A:44:THR:OG1	1:A:127:SER:HA	2.14	0.48
1:B:144:GLU:OE2	1:B:144:GLU:HA	2.13	0.48
2:C:140:TRP:NE1	2:C:145:ILE:HD11	2.29	0.48
2:D:192:MET:HE3	2:D:280:PHE:HD2	1.78	0.48
1:A:413:HIS:HD2	1:A:428:SER:OG	1.97	0.47
2:D:245:ALA:HB3	2:D:299:TYR:OH	2.13	0.47
3:E:44:ARG:HD3	3:E:47:TYR:CZ	2.49	0.47
2:C:98:HIS:HD2	2:C:297:ASP:OD1	1.96	0.47
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.96	0.47
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.97	0.47
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.95	0.47
1:B:196:ASP:HB2	3:F:140:MET:SD	2.55	0.47
1:A:116:ASN:CG	1:A:189:SER:HA	2.40	0.47
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.50	0.47
1:A:403:ILE:HD12	1:A:515:LEU:CD1	2.44	0.47
2:C:203:ILE:HG13	2:C:204:VAL:HG23	1.95	0.47
1:A:417:ILE:HD12	1:A:468:ASN:HB2	1.96	0.47
1:A:521:ASN:OD1	1:A:523:VAL:HG12	2.15	0.47
1:A:165:PRO:HG3	7:A:2807:HOH:O	2.15	0.47
1:A:268:ASN:HD21	1:A:327:GLU:N	2.08	0.47
1:A:461:PRO:HG2	3:E:159:ARG:CZ	2.45	0.47
2:D:357:TYR:CE1	2:D:381:VAL:HG11	2.50	0.47
1:B:43:ARG:HD2	1:B:43:ARG:C	2.39	0.47
2:D:54:VAL:O	2:D:55:TYR:HB2	2.14	0.47
1:B:185:LYS:O	1:B:189:SER:HB2	2.15	0.47
3:E:40:THR:C	3:E:41:THR:HG23	2.39	0.47
1:B:79:PHE:O	1:B:83:GLN:HG3	2.14	0.47
1:B:33:GLN:HA	1:B:33:GLN:HE21	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:PHE:O	1:A:112:VAL:HG12	2.15	0.46
1:B:323:LYS:HE2	1:B:324:TYR:CE1	2.50	0.46
1:A:163:GLN:O	2:C:28:PRO:HA	2.16	0.46
1:A:417:ILE:HD11	1:A:469:ILE:HG12	1.97	0.46
2:D:277:THR:HG22	2:D:281:ILE:CD1	2.45	0.46
3:F:39:HIS:HD2	7:F:191:HOH:O	1.97	0.46
2:C:54:VAL:O	2:C:55:TYR:HB2	2.15	0.46
2:D:324:TRP:HA	2:D:327:PRO:HD2	1.98	0.46
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.51	0.46
1:A:230:GLU:C	1:A:233:PRO:HD2	2.41	0.46
1:B:115:TYR:OH	2:D:173:ASP:HA	2.16	0.46
1:B:460:GLU:N	1:B:461:PRO:HD3	2.30	0.46
2:D:329:ILE:CD1	2:D:380:ILE:HG23	2.46	0.46
3:E:98:MET:HE2	3:E:138:ARG:HG2	1.97	0.46
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.50	0.46
1:B:472:GLN:NE2	7:B:2843:HOH:O	2.49	0.45
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.51	0.45
1:A:291:GLU:OE1	1:A:343:HIS:HE1	2.00	0.45
1:B:175:ARG:HA	1:B:358:PHE:CD2	2.52	0.45
2:C:364:ILE:HA	2:C:368:ALA:HB3	1.98	0.45
1:A:79:PHE:O	1:A:83:GLN:HG3	2.16	0.45
3:F:39:HIS:CD2	3:F:49:LEU:HD12	2.52	0.45
1:A:206:LEU:HD11	1:A:321:LEU:HD11	1.99	0.45
1:A:318:ILE:HG23	1:A:319:GLY:N	2.32	0.45
2:D:223:VAL:HG23	7:D:489:HOH:O	2.16	0.44
1:B:344:HIS:HE1	1:B:376:TYR:CE2	2.36	0.44
1:B:125:TRP:CD1	1:B:125:TRP:C	2.95	0.44
1:B:461:PRO:HG2	3:F:159:ARG:CZ	2.48	0.44
2:C:118:ARG:NH2	2:D:111:LYS:HD3	2.31	0.44
1:B:343:HIS:H	1:B:343:HIS:CD2	2.36	0.44
2:D:153:LEU:HB3	2:D:193:ILE:HG21	2.00	0.44
2:D:349:LYS:O	2:D:352:ILE:HG13	2.17	0.44
3:F:32:LEU:HA	3:F:60:LEU:HD23	1.99	0.44
1:B:212:PHE:C	1:B:215:PRO:HD2	2.41	0.44
1:B:281:TYR:CE1	1:B:285:VAL:HG21	2.52	0.44
2:C:336:MET:HE2	2:C:385:LEU:HD23	1.96	0.44
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.53	0.44
2:D:243:GLU:HB2	2:D:320:TRP:CZ2	2.53	0.44
3:F:4:LEU:HD21	3:F:10:ASP:H	1.81	0.44
1:A:24:ASN:OD1	1:A:26:GLN:CG	2.63	0.44
1:B:268:ASN:ND2	1:B:327:GLU:H	2.08	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:108:GLU:O	3:F:112:ILE:HG12	2.18	0.44
1:A:343:HIS:CD2	1:A:343:HIS:H	2.35	0.44
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.99	0.44
1:A:188:PHE:CE1	1:A:282:PHE:HZ	2.35	0.44
1:A:246:HIS:N	1:A:246:HIS:CD2	2.86	0.44
2:D:98:HIS:HD2	2:D:297:ASP:OD1	2.00	0.44
2:D:184:PHE:O	2:D:187:ILE:HG22	2.18	0.44
2:D:277:THR:O	2:D:281:ILE:HD13	2.18	0.44
1:A:89:LEU:HD21	1:B:230:GLU:HG3	2.00	0.43
1:B:471:GLU:HB3	7:F:201:HOH:O	2.18	0.43
2:D:192:MET:HE3	2:D:280:PHE:CE2	2.53	0.43
1:A:125:TRP:HE1	2:C:161:ASN:HD22	1.66	0.43
1:A:303:LYS:HE3	1:A:303:LYS:HB2	1.87	0.43
1:B:78:GLN:HE21	1:B:235:VAL:HA	1.84	0.43
2:D:349:LYS:HA	2:D:352:ILE:HG13	2.01	0.43
1:A:83:GLN:HB3	1:B:77:ARG:NH1	2.31	0.43
1:A:209:GLU:HA	1:A:213:THR:HB	2.00	0.43
1:B:186:ARG:HA	2:D:73:THR:OG1	2.18	0.43
2:C:3:MET:CG	2:C:4:LEU:N	2.75	0.43
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.83	0.43
1:B:118:ILE:HG21	1:B:145:ILE:HD11	2.01	0.43
1:B:123:MET:SD	2:D:168:ARG:NH1	2.91	0.43
3:F:23:ASN:N	3:F:23:ASN:HD22	2.17	0.43
1:A:360:ARG:HG2	1:A:498:GLN:HB2	2.01	0.43
1:A:437:ARG:NH1	1:A:454:GLU:OE2	2.50	0.43
1:A:81:SER:OG	1:B:84:ASP:HB3	2.18	0.43
1:A:495:LEU:HD11	1:A:512:ILE:CD1	2.47	0.43
1:B:50:TYR:CD1	1:B:50:TYR:N	2.87	0.43
2:C:137:ASN:HA	2:C:138:PRO:HD3	1.88	0.43
1:A:310:TYR:CZ	1:A:336:LYS:HD2	2.53	0.43
1:B:341:TRP:CE2	1:B:431:LYS:HD3	2.54	0.43
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.19	0.43
1:B:291:GLU:OE1	1:B:343:HIS:HE1	2.01	0.43
2:C:259:PHE:CE1	2:C:356:LEU:HD22	2.54	0.43
2:D:349:LYS:HA	2:D:352:ILE:CG1	2.49	0.43
3:F:22:LEU:HD13	3:F:28:ALA:HA	2.00	0.43
3:F:23:ASN:HD22	3:F:23:ASN:C	2.26	0.43
2:C:277:THR:HB	2:C:278:PRO:HD3	2.01	0.43
2:D:169:GLU:O	2:D:170:ALA:C	2.60	0.43
3:E:98:MET:HE1	3:E:107:ALA:HB1	1.99	0.43
3:F:125:VAL:HG23	3:F:126:ASN:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LEU:O	1:A:220:VAL:HG23	2.18	0.42
1:A:360:ARG:NH2	1:A:501:VAL:O	2.52	0.42
1:A:466:CYS:HB2	2:C:73:THR:HA	2.00	0.42
1:A:472:GLN:NE2	7:A:2800:HOH:O	2.52	0.42
2:C:50:GLU:OE1	2:C:99:ARG:NH1	2.52	0.42
2:D:189:ILE:HD11	2:D:287:TYR:CD1	2.54	0.42
3:F:118:TYR:HB3	3:F:123:MET:HB2	2.00	0.42
1:B:260:ASP:OD2	1:B:262:ALA:HB3	2.19	0.42
1:B:397:ASP:HA	1:B:398:PRO:HD3	1.85	0.42
2:D:291:ALA:O	2:D:295:VAL:HG23	2.20	0.42
1:A:365:ASP:OD2	1:A:365:ASP:C	2.62	0.42
1:B:140:GLN:HG3	1:B:246:HIS:CE1	2.54	0.42
2:D:145:ILE:HD11	2:D:274:ASP:OD2	2.19	0.42
1:A:108:ASN:HD21	1:A:175:ARG:HE	1.67	0.42
2:D:82:SER:O	2:D:168:ARG:NH2	2.50	0.42
2:D:98:HIS:CD2	2:D:99:ARG:H	2.37	0.42
3:F:74:GLU:O	3:F:78:ARG:HG3	2.19	0.42
1:A:149:HIS:CE1	2:C:105:TRP:HB2	2.55	0.42
1:B:204:LEU:HG	1:B:205:GLN:HG3	2.02	0.42
2:D:185:ASP:O	2:D:189:ILE:HG12	2.20	0.42
1:A:184:MET:HE3	1:A:184:MET:HA	2.01	0.42
2:C:324:TRP:C	2:C:327:PRO:HD2	2.45	0.42
2:D:376:ASP:OD2	2:D:379:GLN:HG2	2.20	0.42
1:A:435:THR:HG21	1:A:437:ARG:NE	2.34	0.42
1:B:466:CYS:HB2	2:D:73:THR:HA	2.02	0.42
3:F:32:LEU:HD13	3:F:60:LEU:HB3	2.02	0.42
1:B:159:ALA:O	2:D:33:ASN:HB2	2.20	0.42
1:A:204:LEU:O	1:A:209:GLU:HG3	2.19	0.42
1:B:18:ARG:O	2:D:129:ALA:HA	2.19	0.42
1:A:283:THR:HB	1:A:284:PRO:HD3	2.01	0.41
1:A:352:ALA:HA	1:A:404:PRO:CB	2.34	0.41
1:B:188:PHE:CE1	1:B:282:PHE:HZ	2.39	0.41
1:B:232:THR:HB	1:B:233:PRO:HD3	2.02	0.41
2:C:347:THR:HG21	2:C:352:ILE:HD11	2.02	0.41
2:D:213:VAL:HG23	7:D:502:HOH:O	2.20	0.41
1:A:108:ASN:O	1:A:111:GLU:HB3	2.20	0.41
1:A:313:TRP:C	1:A:315:GLY:H	2.28	0.41
1:B:184:MET:HE2	1:B:188:PHE:CD2	2.55	0.41
1:B:246:HIS:CD2	1:B:246:HIS:N	2.87	0.41
1:B:292:TYR:OH	1:B:344:HIS:CD2	2.71	0.41
2:D:63:ILE:O	2:D:64:ALA:C	2.62	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:90:LEU:CD1	2:D:303:LEU:HD13	2.45	0.41
1:B:313:TRP:CZ2	1:B:318:ILE:HD11	2.55	0.41
1:A:146:ARG:HB2	2:C:106:HIS:CE1	2.55	0.41
1:B:41:ASN:O	2:D:236:GLN:HB3	2.21	0.41
2:D:300:TYR:CE1	2:D:370:ARG:HG3	2.55	0.41
2:C:16:MET:O	2:C:20:ILE:HG12	2.20	0.41
2:D:143:GLU:O	2:D:147:ARG:HB3	2.20	0.41
3:E:165:HIS:CE1	3:E:167:GLN:HG3	2.56	0.41
1:A:121:THR:HG21	1:A:140:GLN:CG	2.51	0.41
1:B:108:ASN:ND2	1:B:175:ARG:HH21	2.19	0.41
3:E:12:ARG:O	3:E:16:VAL:HG23	2.21	0.41
1:A:302:VAL:CG1	1:A:376:TYR:HE2	2.28	0.41
1:B:521:ASN:OD1	1:B:523:VAL:HG12	2.20	0.41
2:D:98:HIS:HA	2:D:302:CYS:SG	2.60	0.41
1:A:212:PHE:O	1:A:215:PRO:HD2	2.20	0.41
1:B:288:MET:CE	1:B:347:TYR:N	2.80	0.41
3:E:44:ARG:NH2	3:E:50:ASP:OD1	2.54	0.41
1:A:93:VAL:HG11	2:D:3:MET:HG2	2.02	0.41
1:A:299:GLU:CG	1:A:303:LYS:HD3	2.51	0.41
1:B:460:GLU:OE1	1:B:463:ARG:HD3	2.21	0.41
2:C:9:ARG:NH2	7:C:591:HOH:O	2.48	0.41
2:C:99:ARG:HH11	2:C:99:ARG:HG3	1.86	0.41
2:D:155:ASN:ND2	2:D:252:TYR:OH	2.53	0.41
2:C:347:THR:CG2	2:C:352:ILE:HD11	2.51	0.41
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.56	0.40
1:A:435:THR:CG2	1:A:437:ARG:NE	2.81	0.40
1:A:460:GLU:N	1:A:461:PRO:HD3	2.36	0.40
1:B:109:PHE:O	1:B:112:VAL:HG12	2.21	0.40
1:B:165:PRO:HG3	7:B:2850:HOH:O	2.21	0.40
2:D:137:ASN:HA	2:D:138:PRO:HD3	1.92	0.40
2:D:179:LEU:HD23	2:D:182:TRP:CE3	2.56	0.40
1:A:118:ILE:HG21	1:A:145:ILE:HD11	2.03	0.40
1:A:397:ASP:HA	1:A:398:PRO:HD3	1.80	0.40
2:D:105:TRP:O	2:D:108:PRO:HD2	2.20	0.40
3:F:40:THR:O	3:F:41:THR:OG1	2.37	0.40
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.21	0.40
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.56	0.40
1:B:190:ASP:HB3	2:D:74:GLN:O	2.21	0.40
3:F:23:ASN:N	3:F:23:ASN:ND2	2.69	0.40
2:C:3:MET:HE2	2:C:4:LEU:HD13	2.02	0.40
2:D:255:LEU:HB2	2:D:328:THR:HG21	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:153:GLU:H	3:E:153:GLU:CD	2.30	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%)	484 (95%)	24 (5%)	0	100	100
1	B	508/527 (96%)	484 (95%)	23 (4%)	1 (0%)	43	36
2	C	386/389 (99%)	375 (97%)	10 (3%)	1 (0%)	36	28
2	D	386/389 (99%)	366 (95%)	16 (4%)	4 (1%)	12	5
3	E	164/170 (96%)	161 (98%)	3 (2%)	0	100	100
3	F	164/170 (96%)	157 (96%)	6 (4%)	1 (1%)	21	12
All	All	2116/2172 (97%)	2027 (96%)	82 (4%)	7 (0%)	36	28

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	LYS
2	D	64	ALA
2	D	205	PRO
2	C	251	VAL
2	D	251	VAL
2	D	221	GLY
3	F	6	ILE

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%)	413 (98%)	10 (2%)	43	36
1	B	422/442 (96%)	412 (98%)	10 (2%)	43	36
2	C	315/323 (98%)	310 (98%)	5 (2%)	55	52
2	D	312/323 (97%)	307 (98%)	5 (2%)	55	52
3	E	143/147 (97%)	141 (99%)	2 (1%)	59	56
3	F	142/147 (97%)	137 (96%)	5 (4%)	32	22
All	All	1757/1824 (96%)	1720 (98%)	37 (2%)	47	41

All (37) 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	125	TRP
1	A	175	ARG
1	A	310	TYR
1	A	318	ILE
1	A	391	ARG
1	A	403	ILE
1	A	467	GLN
1	B	30	ARG
1	B	33	GLN
1	B	90	ASN
1	B	110	LEU
1	B	125	TRP
1	B	247	MET
1	B	279	GLN
1	B	310	TYR
1	B	311	GLU
1	B	334	ASP
2	C	33	ASN
2	C	153	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	173	ASP
2	C	356	LEU
2	C	377	ARG
2	D	4	LEU
2	D	80	ARG
2	D	173	ASP
2	D	205	PRO
2	D	371	ILE
3	E	24	THR
3	E	44	ARG
3	F	11	THR
3	F	23	ASN
3	F	44	ARG
3	F	164	VAL
3	F	167	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	78	GLN
1	A	83	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	343	HIS
1	A	344	HIS
1	A	413	HIS
1	A	439	HIS
1	A	442	ASN
1	A	472	GLN
1	A	486	HIS
1	A	516	ASN
1	B	33	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	36	ASN
1	B	78	GLN
1	B	83	GLN
1	B	90	ASN
1	B	100	ASN
1	B	108	ASN
1	B	129	GLN
1	B	133	GLN
1	B	168	HIS
1	B	205	GLN
1	B	227	ASN
1	B	249	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	439	HIS
1	B	451	GLN
1	B	472	GLN
1	B	516	ASN
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	293	GLN
2	D	296	GLN
2	D	301	ASN
3	E	23	ASN
3	E	34	GLN
3	E	45	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	144	ASN
3	F	167	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 8 ligands modelled in this entry, 4 are monoatomic and 2 are modelled with single atom - leaving 2 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	IPH	B	2666	-	7,7,7	2.43	3 (42%)	8,8,8	1.88	2 (25%)
6	IPH	A	2667	-	7,7,7	2.39	3 (42%)	8,8,8	1.85	2 (25%)

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	IPH	B	2666	-	-	-	0/1/1/1
6	IPH	A	2667	-	-	-	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2666	IPH	C5-C6	3.94	1.45	1.38
6	A	2667	IPH	C5-C6	3.77	1.45	1.38
6	B	2666	IPH	C3-C2	3.46	1.44	1.38
6	A	2667	IPH	C3-C2	3.39	1.44	1.38
6	B	2666	IPH	C2-C1	2.47	1.43	1.39
6	A	2667	IPH	C2-C1	2.39	1.43	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	2666	IPH	C6-C1-C2	3.69	125.64	119.77
6	A	2667	IPH	C6-C1-C2	3.62	125.52	119.77
6	B	2666	IPH	C3-C2-C1	-2.49	115.93	119.29
6	A	2667	IPH	C3-C2-C1	-2.47	115.95	119.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	510/527 (96%)	0.09	13 (2%) 58 65	12, 21, 37, 48	0
1	B	510/527 (96%)	0.19	21 (4%) 41 48	13, 23, 37, 49	0
2	C	388/389 (99%)	-0.32	4 (1%) 79 84	10, 16, 29, 44	0
2	D	388/389 (99%)	0.92	62 (15%) 5 5	17, 30, 49, 77	0
3	E	166/170 (97%)	-0.02	7 (4%) 40 47	13, 19, 31, 54	0
3	F	166/170 (97%)	1.64	52 (31%) 1 0	26, 39, 55, 64	0
All	All	2128/2172 (97%)	0.30	159 (7%) 20 23	10, 23, 44, 77	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	385	LEU	6.3
2	D	352	ILE	5.8
3	F	4	LEU	5.6
3	E	4	LEU	5.4
3	F	19	ILE	4.8
2	D	380	ILE	4.7
2	C	3	MET	4.6
2	D	371	ILE	4.6
1	B	403	ILE	4.5
2	D	388	LEU	4.5
2	D	384	VAL	4.4
3	F	20	ALA	4.3
2	D	386	ALA	4.1
1	A	318	ILE	3.9
3	F	83	PHE	3.9
3	F	25	LEU	3.8
3	E	168	SER	3.8
3	F	24	THR	3.8
3	F	23	ASN	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	387	GLY	3.6
2	D	389	LYS	3.6
3	F	22	LEU	3.6
2	D	374	LYS	3.5
2	D	373	PHE	3.5
3	F	82	ALA	3.5
2	D	381	VAL	3.4
3	F	16	VAL	3.4
3	F	72	PHE	3.4
3	F	5	GLY	3.3
2	D	335	PHE	3.3
2	D	372	ASP	3.3
3	F	69	ALA	3.3
2	D	347	THR	3.3
1	B	54	ASN	3.3
1	B	316	ILE	3.2
3	F	11	THR	3.2
2	D	379	GLN	3.2
2	D	357	TYR	3.2
3	F	75	VAL	3.2
1	A	317	TRP	3.1
3	F	28	ALA	3.1
1	A	310	TYR	3.1
1	B	258	ALA	3.1
3	F	71	ALA	3.1
3	E	3	LYS	3.0
2	D	368	ALA	3.0
3	F	66	VAL	3.0
3	F	80	LYS	3.0
2	D	332	LEU	2.9
3	F	67	LEU	2.9
3	F	163	VAL	2.9
1	A	18	ARG	2.9
2	D	363	TRP	2.9
2	D	344	ALA	2.9
2	C	4	LEU	2.9
1	A	54	ASN	2.9
2	D	376	ASP	2.9
1	B	525	ALA	2.8
3	F	60	LEU	2.8
3	F	161	VAL	2.8
1	B	517	CYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	E	23	ASN	2.8
2	D	337	GLY	2.8
2	D	329	ILE	2.8
3	F	164	VAL	2.8
3	F	118	TYR	2.7
2	D	230	ALA	2.7
3	F	64	VAL	2.7
1	B	317	TRP	2.7
2	D	338	LEU	2.7
2	D	205	PRO	2.7
3	F	122	ILE	2.7
3	F	81	THR	2.7
1	B	256	SER	2.7
3	F	125	VAL	2.7
2	D	331	ALA	2.6
2	D	330	ALA	2.6
3	E	167	GLN	2.6
2	D	264	PHE	2.6
2	D	336	MET	2.6
1	B	53	ALA	2.6
2	D	227	ALA	2.6
2	D	316	VAL	2.6
2	C	205	PRO	2.6
2	D	354	ALA	2.6
2	D	339	PHE	2.5
2	D	320	TRP	2.5
2	D	216	ALA	2.5
1	A	213	THR	2.5
3	F	70	ARG	2.5
3	F	84	GLY	2.5
2	D	383	ALA	2.5
2	D	270	PRO	2.5
2	D	206	GLY	2.4
3	F	78	ARG	2.4
1	B	259	ASN	2.4
2	D	281	ILE	2.4
1	B	310	TYR	2.3
1	B	213	THR	2.3
1	B	311	GLU	2.3
3	F	96	ALA	2.3
1	B	44	THR	2.3
3	F	127	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	79	HIS	2.3
3	F	101	ALA	2.3
1	A	302	VAL	2.3
2	D	348	ASP	2.3
3	F	21	GLN	2.3
2	D	328	THR	2.3
3	F	31	MET	2.3
1	B	39	PHE	2.3
2	D	340	ALA	2.3
1	A	403	ILE	2.3
1	A	76	GLU	2.3
3	F	30	GLU	2.3
2	D	148	TYR	2.2
2	D	224	TYR	2.2
3	F	77	PHE	2.2
3	F	120	PRO	2.2
2	D	375	ALA	2.2
1	B	480	GLU	2.2
3	F	85	GLU	2.2
3	E	22	LEU	2.2
2	D	345	GLY	2.2
3	F	29	ALA	2.2
1	A	316	ILE	2.2
1	B	257	ILE	2.2
3	F	112	ILE	2.2
2	D	361	ASP	2.2
2	D	229	LEU	2.2
3	F	100	ALA	2.2
2	D	341	LYS	2.2
1	B	70	MET	2.1
3	E	31	MET	2.1
3	F	26	GLU	2.1
3	F	15	TRP	2.1
2	D	360	VAL	2.1
2	D	377	ARG	2.1
3	F	32	LEU	2.1
2	C	389	LYS	2.1
1	A	389	GLU	2.1
1	B	76	GLU	2.1
3	F	17	ASN	2.1
3	F	114	PHE	2.1
2	D	367	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	320	ARG	2.1
2	D	370	ARG	2.1
1	B	441	TYR	2.1
2	D	356	LEU	2.1
1	A	19	ALA	2.1
1	A	319	GLY	2.0
3	F	73	ASN	2.0
2	D	311	ASP	2.0
2	D	333	ARG	2.0
2	D	350	GLU	2.0
3	F	153	GLU	2.0
2	D	310	SER	2.0
2	D	176	ARG	2.0
2	D	213	VAL	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	IPH	A	2667	7/7	0.90	0.15	29,30,31,32	0
6	IPH	B	2666	7/7	0.90	0.12	26,27,29,32	0
5	OH	B	1173	1/1	0.97	0.07	25,25,25,25	0
5	OH	A	1177	1/1	0.98	0.05	23,23,23,23	0
4	FE	A	1175	1/1	0.99	0.03	24,24,24,24	0
4	FE	B	1171	1/1	0.99	0.03	26,26,26,26	0
4	FE	B	1170	1/1	1.00	0.01	19,19,19,19	0
4	FE	A	1174	1/1	1.00	0.01	19,19,19,19	0

6.5 Other polymers ⓘ

There are no such residues in this entry.