



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:47 PM UTC

PDB ID : 9NPN / pdb_00009nnpn
Title : Crystal structure of the inactive conformation of a glycoside hydrolase (CapGH2b - E465A Mutant) from the GH2 family in the space group P1 at 3.1 Å
Authors : Martins, M.P.; Spadeto, J.P.M.; Miyamoto, R.Y.; Morais, M.A.B.; Murakami, M.T.
Deposited on : 2025-03-11
Resolution : 3.10 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

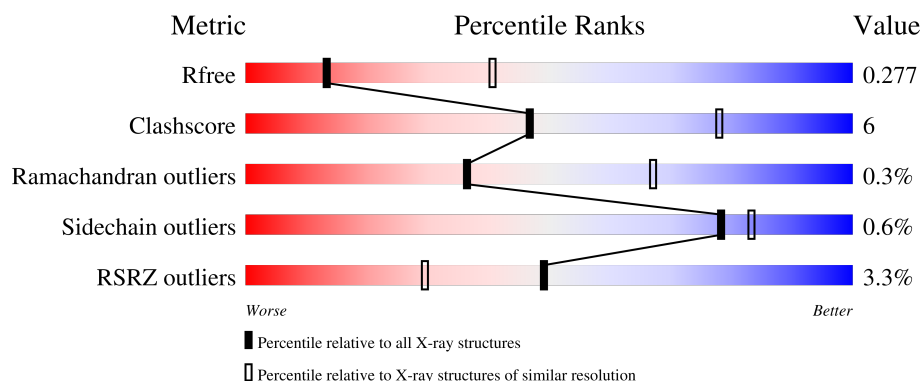
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	798	0% 77% 14% 9%
1	B	798	4% 78% 12% 9%
1	C	798	4% 76% 13% 10%
1	D	798	2% 78% 12% 10%

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Mol	Chain	Length	Quality of chain
1	E	798	2% 80% 11% 9%
1	F	798	6% 71% 15% 12%

2 Entry composition [i](#)

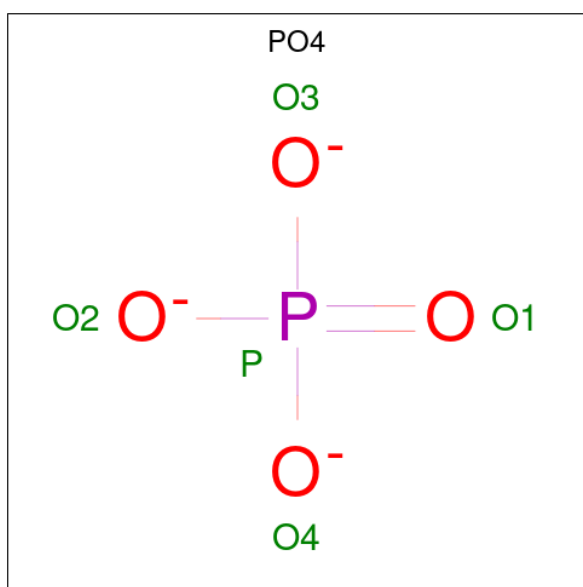
There are 4 unique types of molecules in this entry. The entry contains 35009 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycoside hydrolase family 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	0	0
			5839	3732	998	1080	29			
1	B	725	Total	C	N	O	S	0	0	0
			5830	3725	996	1080	29			
1	C	718	Total	C	N	O	S	0	0	0
			5780	3693	986	1072	29			
1	D	717	Total	C	N	O	S	0	0	0
			5755	3673	985	1068	29			
1	E	726	Total	C	N	O	S	0	0	0
			5841	3735	997	1080	29			
1	F	700	Total	C	N	O	S	0	0	0
			5625	3590	961	1045	29			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	41	Total O 41 41	0	0

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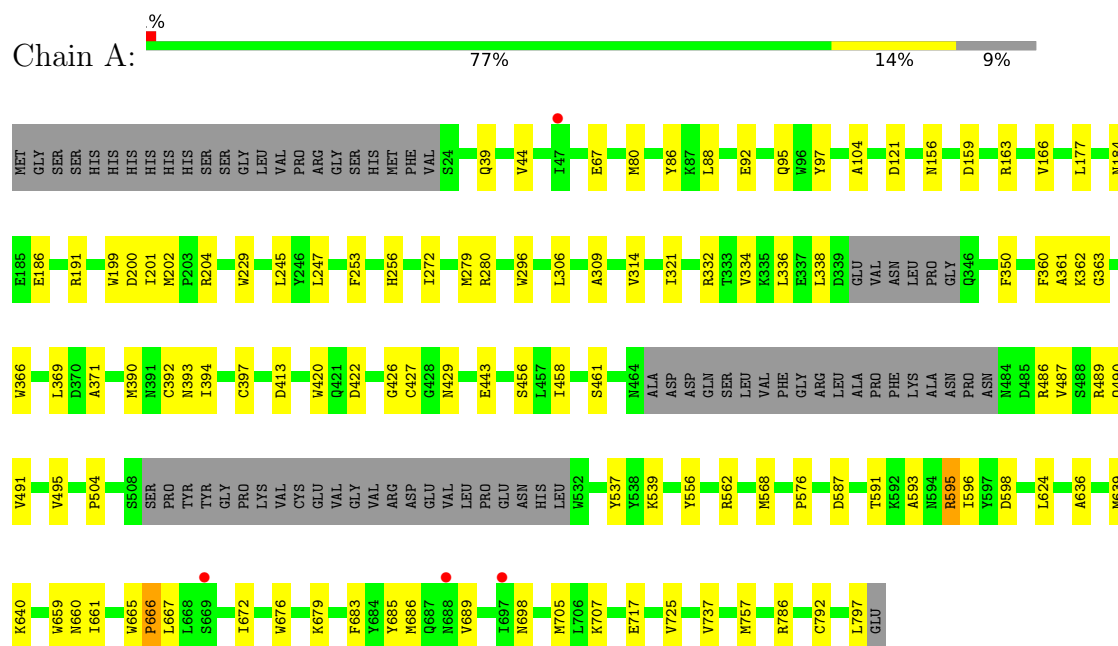
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	28	Total 28	O 28	0	0
4	C	46	Total 46	O 46	0	0
4	D	22	Total 22	O 22	0	0
4	E	31	Total 31	O 31	0	0
4	F	21	Total 21	O 21	0	0

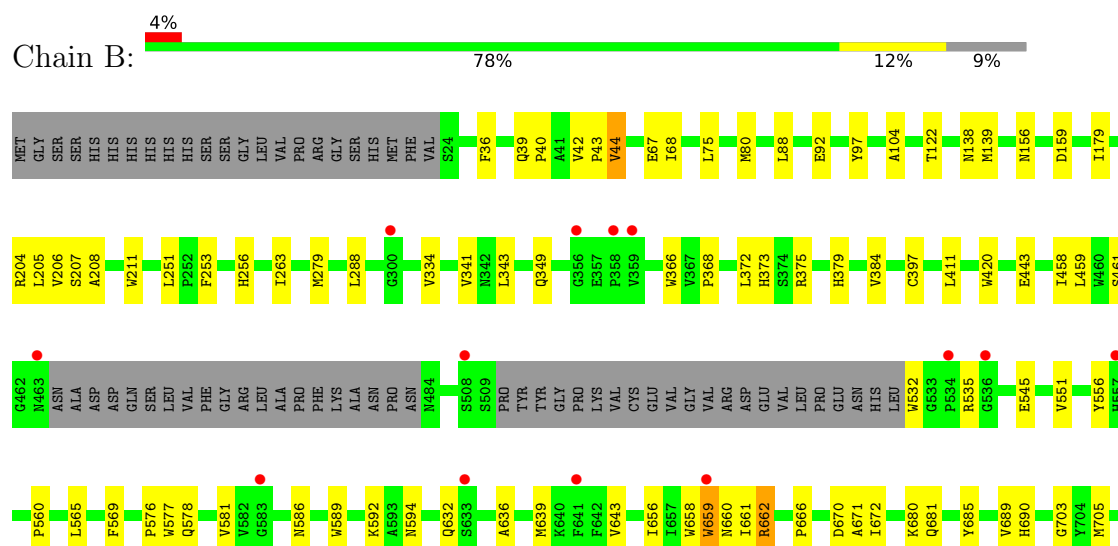
3 Residue-property plots [i](#)

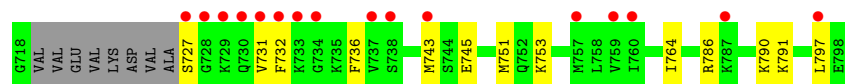
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Glycoside hydrolase family 2

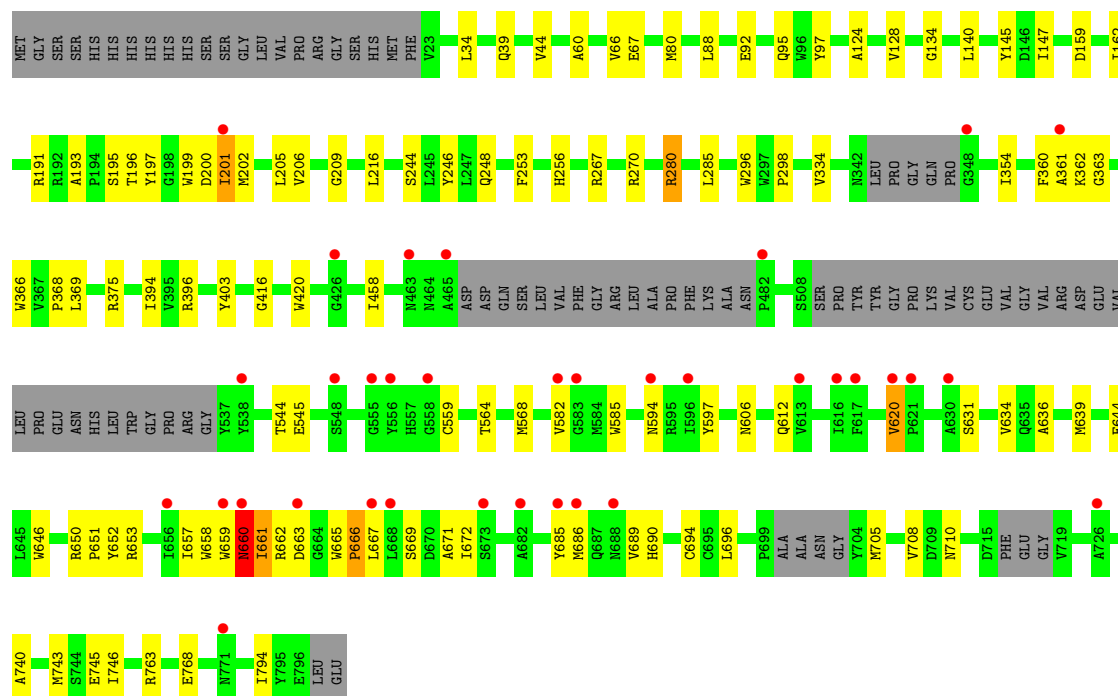
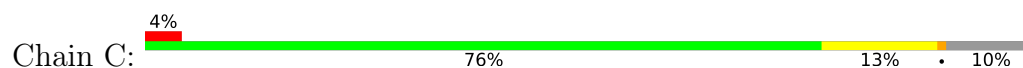


• Molecule 1: Glycoside hydrolase family 2

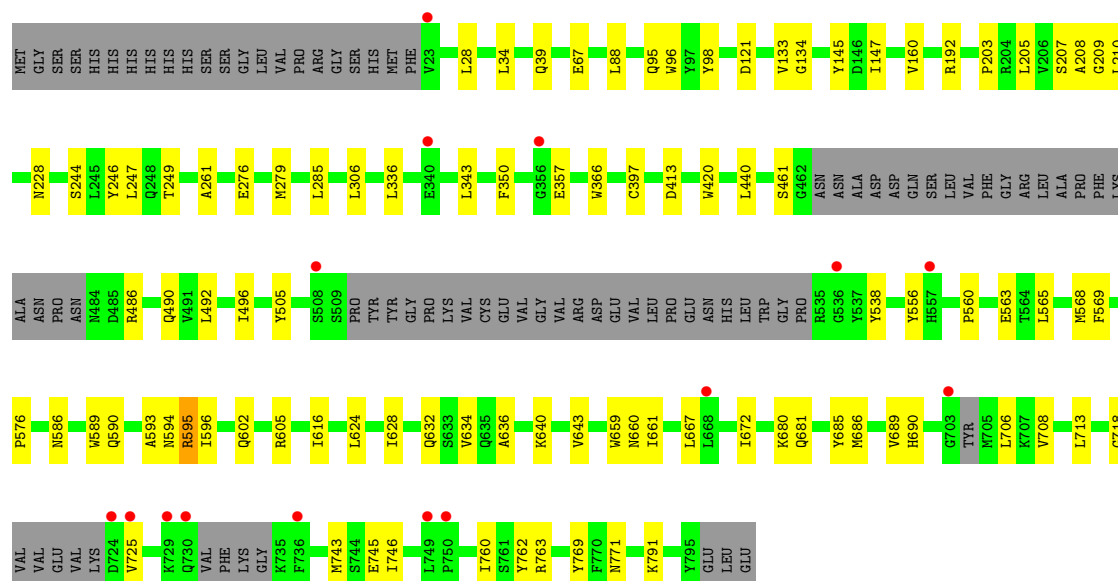
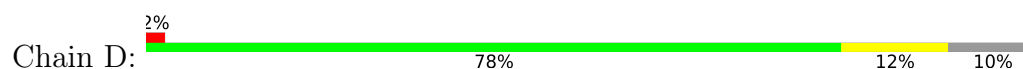




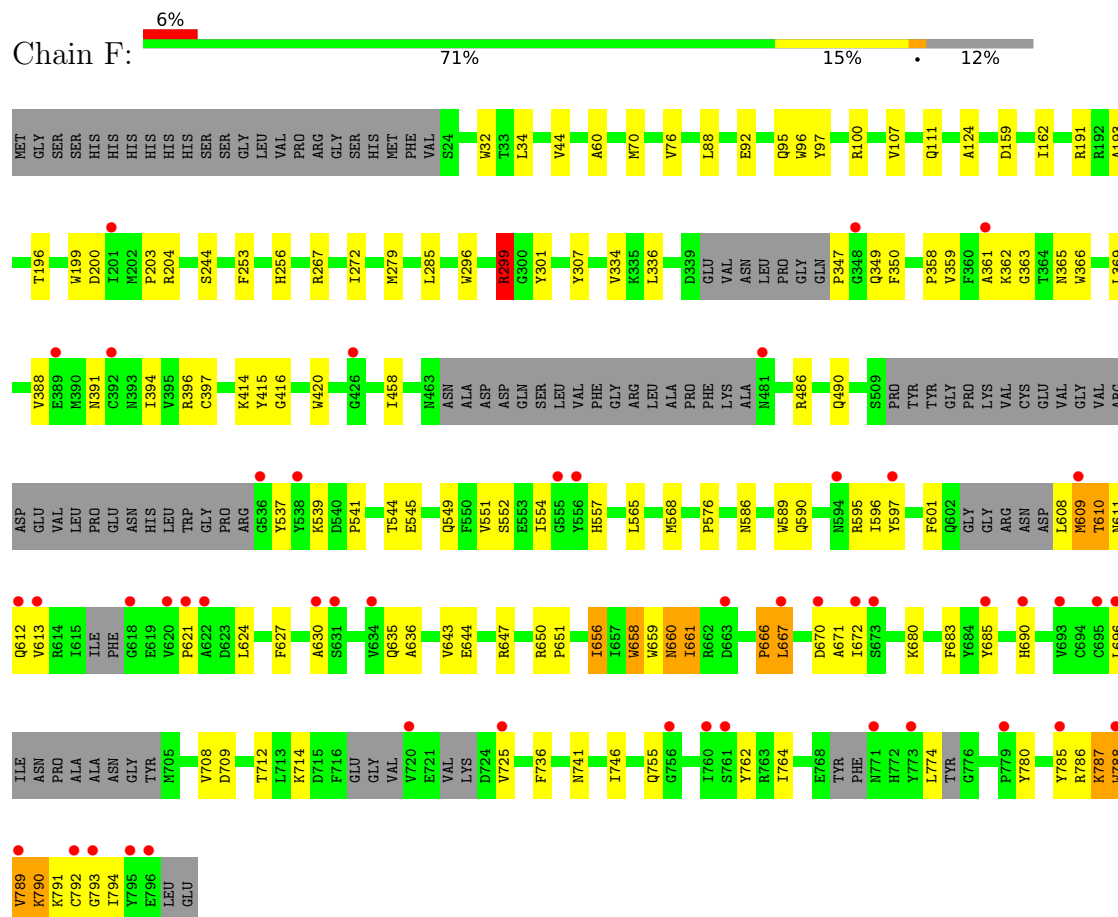
• Molecule 1: Glycoside hydrolase family 2



• Molecule 1: Glycoside hydrolase family 2



• Molecule 1: Glycoside hydrolase family 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	123.28Å 123.72Å 133.04Å 89.13° 117.56° 103.51°	Depositor
Resolution (Å)	49.15 – 3.10 49.15 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.15-3.10) 98.0 (49.15-3.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.245 , 0.276 0.246 , 0.277	Depositor DCC
R_{free} test set	5998 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	66.9	Xtriage
Anisotropy	0.785	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	35009	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.69% 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: PO4, EDO

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	0.31	0/5991	0.49	0/8133
1	B	0.28	0/5983	0.42	2/8122 (0.0%)
1	C	0.30	0/5926	0.46	3/8042 (0.0%)
1	D	0.27	0/5901	0.44	4/8008 (0.0%)
1	E	0.26	0/5993	0.45	4/8135 (0.0%)
1	F	0.28	0/5762	0.43	3/7810 (0.0%)
All	All	0.28	0/35556	0.45	16/48250 (0.0%)

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	4
1	B	0	3
1	C	0	1
1	D	0	2
1	E	0	1
1	F	0	2
All	All	0	13

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	661	ILE	N-CA-C	-9.38	104.00	113.10
1	E	593	ALA	N-CA-C	-8.40	100.12	111.54
1	D	593	ALA	N-CA-C	-7.34	104.27	112.57
1	F	661	ILE	N-CA-C	-7.29	105.48	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	670	ASP	N-CA-C	-6.75	104.92	113.02
1	D	28	LEU	N-CA-C	-6.38	105.08	112.92
1	E	647	ARG	N-CA-C	-5.51	105.81	112.54
1	C	209	GLY	CA-C-O	-5.20	118.71	122.45
1	D	209	GLY	CA-C-O	-5.20	118.71	122.45
1	C	360	PHE	CB-CA-C	-5.14	101.27	109.75
1	E	28	LEU	N-CA-C	-5.12	106.88	113.02
1	B	659	TRP	CA-C-N	-5.04	113.07	121.94
1	B	659	TRP	C-N-CA	-5.04	113.07	121.94
1	E	595	ARG	N-CA-C	-5.04	100.30	108.41
1	F	609	MET	CA-C-O	-5.03	116.15	120.88
1	D	210	LEU	N-CA-CB	-5.03	101.94	109.88

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	ASP	Peptide
1	A	489	ARG	Sidechain
1	A	593	ALA	Peptide
1	A	595	ARG	Sidechain
1	B	204	ARG	Sidechain
1	B	658	TRP	Peptide
1	B	662	ARG	Sidechain
1	C	280	ARG	Sidechain
1	D	595	ARG	Sidechain
1	D	605	ARG	Sidechain
1	E	204	ARG	Sidechain
1	F	299	ARG	Sidechain
1	F	786	ARG	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	5839	0	5660	76	0
1	B	5830	0	5643	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5780	0	5608	71	0
1	D	5755	0	5576	53	0
1	E	5841	0	5665	55	0
1	F	5625	0	5452	84	0
2	A	15	0	0	0	0
2	B	10	0	0	0	0
2	C	30	0	0	0	0
2	D	20	0	0	0	0
2	E	20	0	0	0	0
2	F	15	0	0	0	0
3	A	8	0	12	0	0
3	B	4	0	6	0	0
3	C	4	0	6	0	0
3	D	4	0	6	1	0
3	E	12	0	18	0	0
3	F	8	0	12	0	0
4	A	41	0	0	0	0
4	B	28	0	0	0	0
4	C	46	0	0	0	0
4	D	22	0	0	0	0
4	E	31	0	0	0	0
4	F	21	0	0	0	0
All	All	35009	0	33664	393	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 6.

All (393) 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:384:VAL:HG21	1:B:411:LEU:HD23	1.80	0.64
1:C:201:ILE:O	1:C:201:ILE:HG22	1.98	0.63
1:C:80:MET:HB3	1:C:666:PRO:HG2	1.79	0.63
1:A:556:TYR:HB2	1:A:639:MET:HE3	1.81	0.63
1:A:177:LEU:HD13	1:A:429:ASN:HD22	1.63	0.63
1:F:347:PRO:HG2	1:F:551:VAL:HA	1.80	0.62
1:A:576:PRO:HD3	1:A:624:LEU:HD13	1.80	0.62
1:F:762:TYR:HD2	1:F:764:ILE:HD11	1.64	0.62
1:A:245:LEU:HD21	1:A:247:LEU:HB2	1.81	0.61
1:C:201:ILE:O	1:C:201:ILE:CG2	2.47	0.61
1:E:113:LEU:HD13	1:E:151:VAL:HG11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:420:TRP:HE1	1:D:461:SER:HB2	1.65	0.61
1:F:568:MET:HG2	1:F:666:PRO:HB3	1.82	0.61
1:E:105:PRO:HD2	1:E:113:LEU:HD11	1.83	0.60
1:B:790:LYS:HD3	1:B:797:LEU:HD11	1.84	0.60
1:E:27:SER:OG	1:E:29:ASN:HB2	2.02	0.60
1:C:661:ILE:HG13	1:C:672:ILE:HD11	1.84	0.60
1:B:703:GLY:HA2	1:B:751:MET:HB2	1.84	0.60
1:B:751:MET:HE3	1:B:753:LYS:HE2	1.84	0.59
1:D:366:TRP:HB3	1:D:397:CYS:HA	1.84	0.59
1:E:262:VAL:HG12	1:E:276:GLU:HG2	1.85	0.59
1:F:672:ILE:HD12	1:F:683:PHE:HA	1.85	0.59
1:F:554:ILE:HG22	1:F:658:TRP:HA	1.85	0.59
1:A:725:VAL:HG23	1:A:757:MET:O	2.03	0.59
1:B:42:VAL:O	1:B:42:VAL:HG13	2.02	0.58
1:B:420:TRP:CE2	1:B:459:LEU:HD23	2.38	0.58
1:E:650:ARG:O	1:E:651:PRO:C	2.45	0.58
1:F:299:ARG:HG2	1:F:299:ARG:HH11	1.67	0.58
1:C:201:ILE:HD13	1:C:659:TRP:HE1	1.68	0.58
1:F:486:ARG:O	1:F:490:GLN:HB2	2.03	0.58
1:A:360:PHE:O	1:A:393:ASN:ND2	2.35	0.58
1:C:34:LEU:HB2	1:C:60:ALA:HB2	1.84	0.58
1:F:608:LEU:O	1:F:609:MET:C	2.45	0.58
1:C:201:ILE:HG12	1:C:669:SER:HB2	1.85	0.58
1:C:644:GLU:HG2	1:C:696:LEU:HD22	1.86	0.58
1:C:650:ARG:HB3	1:C:743:MET:HB2	1.86	0.58
1:B:661:ILE:HA	1:B:672:ILE:HG12	1.85	0.58
1:E:204:ARG:HB2	1:E:596:ILE:HG23	1.86	0.57
1:C:34:LEU:HD11	1:C:66:VAL:HG12	1.86	0.57
1:B:532:TRP:HB3	1:B:535:ARG:HE	1.68	0.57
1:E:366:TRP:HB3	1:E:397:CYS:HA	1.85	0.57
1:B:556:TYR:HB2	1:B:639:MET:HE3	1.87	0.57
1:B:659:TRP:HD1	1:B:670:ASP:OD1	1.87	0.57
1:A:568:MET:HG3	1:A:676:TRP:HZ3	1.68	0.57
1:B:689:VAL:HG12	1:B:689:VAL:O	2.04	0.57
1:C:705:MET:HE3	1:C:745:GLU:HB3	1.87	0.57
1:F:636:ALA:HB1	1:F:685:TYR:CG	2.40	0.57
1:B:366:TRP:HB3	1:B:397:CYS:HA	1.86	0.56
1:F:365:ASN:HD22	1:F:659:TRP:HE3	1.54	0.56
1:A:80:MET:HB3	1:A:666:PRO:HG3	1.88	0.56
1:F:790:LYS:HE3	1:F:793:GLY:HA3	1.87	0.56
1:D:640:LYS:HG3	1:D:689:VAL:HG11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:MET:CE	1:A:683:PHE:CE1	2.88	0.56
1:C:201:ILE:HD13	1:C:659:TRP:NE1	2.21	0.55
1:F:590:GLN:HB2	1:F:595:ARG:HH21	1.71	0.55
1:A:366:TRP:HB3	1:A:397:CYS:HA	1.87	0.55
1:B:92:GLU:HB2	1:C:253:PHE:CZ	2.42	0.55
1:E:310:GLU:HG3	1:E:326:THR:HG22	1.87	0.55
1:F:44:VAL:HB	1:F:95:GLN:HE22	1.70	0.55
1:A:296:TRP:HB3	1:A:332:ARG:HB3	1.88	0.55
1:D:121:ASP:OD1	1:D:192:ARG:NH1	2.40	0.55
1:B:80:MET:HE2	1:B:375:ARG:HH22	1.71	0.55
1:F:361:ALA:HB1	1:F:394:ILE:HG21	1.89	0.55
1:F:613:VAL:HG23	1:F:613:VAL:O	2.07	0.55
1:A:204:ARG:HB2	1:A:596:ILE:HG23	1.88	0.54
1:B:80:MET:HB3	1:B:666:PRO:HG2	1.89	0.54
1:F:621:PRO:HG2	1:F:627:PHE:HA	1.90	0.54
1:B:104:ALA:HB2	1:B:156:ASN:HD21	1.72	0.54
1:A:361:ALA:HA	1:A:393:ASN:HD21	1.73	0.54
1:A:390:MET:HE1	1:A:683:PHE:CD1	2.43	0.54
1:B:368:PRO:HB3	1:B:373:HIS:HE1	1.73	0.54
1:E:659:TRP:CD1	1:E:660:ASN:HD22	2.26	0.54
1:A:97:TYR:HE1	1:A:159:ASP:HB3	1.73	0.54
1:A:104:ALA:HB2	1:A:156:ASN:HD21	1.72	0.54
1:B:660:ASN:HB3	1:B:671:ALA:HA	1.88	0.54
1:D:67:GLU:HG2	1:D:88:LEU:HD13	1.90	0.54
1:C:636:ALA:HB1	1:C:685:TYR:CG	2.44	0.53
1:E:556:TYR:HB2	1:E:639:MET:HE3	1.89	0.53
1:F:644:GLU:HG2	1:F:696:LEU:HD22	1.90	0.53
1:D:632:GLN:HB3	1:D:681:GLN:HB2	1.90	0.53
1:B:420:TRP:HE1	1:B:461:SER:HB2	1.73	0.53
1:C:97:TYR:HE1	1:C:159:ASP:HB3	1.74	0.53
1:C:147:ILE:HD11	1:C:216:LEU:HD21	1.90	0.53
1:C:362:LYS:HB2	1:C:690:HIS:CE1	2.43	0.53
1:D:616:ILE:HD12	1:D:634:VAL:HG23	1.91	0.53
1:D:725:VAL:HG11	1:D:791:LYS:HB3	1.90	0.53
1:F:789:VAL:HG13	1:F:794:ILE:HG13	1.90	0.53
1:A:686:MET:HA	1:A:689:VAL:HG22	1.91	0.53
1:D:357:GLU:HG2	1:D:713:LEU:HD21	1.90	0.53
1:B:545:GLU:HB3	1:E:239:ARG:HH11	1.74	0.53
1:C:650:ARG:O	1:C:651:PRO:C	2.52	0.53
1:F:193:ALA:HB3	1:F:196:THR:HG23	1.91	0.53
1:E:201:ILE:CD1	1:E:659:TRP:HZ2	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:785:TYR:C	1:F:787:LYS:N	2.65	0.52
1:A:717:GLU:HG2	1:A:737:VAL:HG12	1.92	0.52
1:C:639:MET:HE3	1:C:658:TRP:HB2	1.91	0.52
1:C:665:TRP:O	1:C:667:LEU:HG	2.09	0.52
1:A:253:PHE:CZ	1:C:92:GLU:HB2	2.45	0.52
1:D:261:ALA:HB2	1:D:279:MET:HE1	1.91	0.52
1:F:785:TYR:C	1:F:787:LYS:H	2.16	0.52
1:C:280:ARG:HG2	1:C:280:ARG:HH11	1.73	0.52
1:F:347:PRO:HG2	1:F:552:SER:N	2.25	0.52
1:A:562:ARG:HH21	1:A:624:LEU:HD23	1.74	0.52
1:E:29:ASN:HD21	1:E:213:ASP:HA	1.75	0.52
1:B:705:MET:HE3	1:B:745:GLU:HB2	1.92	0.51
1:F:647:ARG:HH21	1:F:709:ASP:HB3	1.75	0.51
1:A:659:TRP:CD1	1:A:660:ASN:HD22	2.28	0.51
1:B:68:ILE:HG13	1:B:372:LEU:HD22	1.92	0.51
1:B:343:LEU:O	1:B:349:GLN:HG3	2.10	0.51
1:A:80:MET:HE2	1:A:676:TRP:CZ2	2.45	0.51
1:D:228:ASN:HB3	1:D:246:TYR:HB2	1.92	0.51
1:E:301:TYR:OH	1:E:650:ARG:NH2	2.43	0.51
1:E:104:ALA:HB2	1:E:156:ASN:HD21	1.75	0.51
1:D:247:LEU:HD21	1:D:249:THR:HG23	1.92	0.51
1:F:610:THR:C	1:F:612:GLN:H	2.17	0.51
1:B:636:ALA:HB1	1:B:685:TYR:CG	2.46	0.51
1:D:247:LEU:HD21	1:D:249:THR:CG2	2.41	0.51
1:D:538:TYR:HE2	1:D:616:ILE:HD11	1.76	0.51
1:B:786:ARG:HG2	1:B:790:LYS:HE2	1.94	0.50
1:A:338:LEU:HD23	1:A:350:PHE:HB3	1.92	0.50
1:B:661:ILE:HG13	1:B:672:ILE:HD11	1.93	0.50
1:D:706:LEU:HG	1:D:746:ILE:HD12	1.92	0.50
1:F:204:ARG:HB2	1:F:596:ILE:HG23	1.92	0.50
1:E:444:ALA:HB1	1:E:495:VAL:HG21	1.93	0.50
1:F:611:ASN:O	1:F:612:GLN:C	2.54	0.50
1:A:705:MET:HG3	1:A:707:LYS:HG3	1.94	0.50
1:B:560:PRO:HA	1:B:680:LYS:HE2	1.94	0.50
1:F:97:TYR:HE1	1:F:159:ASP:HB3	1.76	0.50
1:E:128:VAL:HG12	1:E:129:ASN:HD22	1.75	0.50
1:A:705:MET:HG2	1:A:707:LYS:HE3	1.93	0.49
1:F:544:THR:HG23	1:F:545:GLU:HG3	1.94	0.49
1:F:708:VAL:HG12	1:F:746:ILE:HD11	1.94	0.49
1:C:193:ALA:HB3	1:C:196:THR:HG23	1.93	0.49
1:C:202:MET:HE3	1:C:368:PRO:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:549:GLN:HG2	1:E:652:TYR:CE2	2.47	0.49
1:C:244:SER:HB3	1:C:285:LEU:HD11	1.94	0.49
1:D:659:TRP:CD1	1:D:660:ASN:HD22	2.31	0.49
1:E:201:ILE:HD13	1:E:659:TRP:HZ2	1.76	0.49
1:A:67:GLU:HG2	1:A:88:LEU:HD13	1.93	0.49
1:F:32:TRP:CE2	1:F:100:ARG:HD2	2.47	0.49
1:E:636:ALA:HB1	1:E:685:TYR:CG	2.48	0.49
1:F:76:VAL:HG11	1:F:88:LEU:HD21	1.94	0.49
1:F:124:ALA:HB2	1:F:162:ILE:HG12	1.93	0.49
1:F:347:PRO:HG2	1:F:552:SER:H	1.78	0.49
1:C:660:ASN:HB3	1:C:671:ALA:HA	1.95	0.49
1:F:299:ARG:HH12	1:F:388:VAL:HG13	1.77	0.49
1:D:636:ALA:HB1	1:D:685:TYR:CG	2.48	0.49
1:A:186:GLU:OE1	1:A:204:ARG:NH2	2.42	0.48
1:A:202:MET:HE1	1:A:371:ALA:HA	1.95	0.48
1:C:396:ARG:HA	1:C:420:TRP:HB3	1.95	0.48
1:A:280:ARG:HD2	1:C:597:TYR:CD1	2.48	0.48
1:C:44:VAL:HB	1:C:95:GLN:HE22	1.78	0.48
1:C:763:ARG:HG2	1:C:768:GLU:HA	1.95	0.48
1:F:586:ASN:HD21	1:F:589:TRP:CD1	2.31	0.48
1:A:636:ALA:HB1	1:A:685:TYR:CG	2.48	0.48
1:A:272:ILE:HA	1:D:343:LEU:HD13	1.95	0.48
1:C:67:GLU:HG2	1:C:88:LEU:HD13	1.94	0.48
1:E:407:HIS:O	1:E:408:PHE:C	2.57	0.48
1:F:334:VAL:HG21	1:F:458:ILE:HB	1.93	0.48
1:A:390:MET:CE	1:A:683:PHE:CD1	2.96	0.48
1:C:39:GLN:HB2	1:C:95:GLN:HG3	1.95	0.48
1:C:92:GLU:HG2	1:C:206:VAL:CG2	2.44	0.48
1:C:612:GLN:HB3	1:C:634:VAL:HG21	1.95	0.48
1:F:613:VAL:HG11	1:F:630:ALA:HB1	1.95	0.48
1:A:422:ASP:OD1	1:A:461:SER:HB3	2.14	0.48
1:C:585:TRP:CE2	1:C:606:ASN:HB3	2.48	0.48
1:A:202:MET:HE3	1:A:202:MET:HB3	1.67	0.48
1:B:586:ASN:HD21	1:B:589:TRP:CD1	2.31	0.48
1:C:361:ALA:HB1	1:C:394:ILE:HG21	1.95	0.48
1:E:253:PHE:CZ	1:F:92:GLU:HB2	2.49	0.48
1:F:296:TRP:CZ2	1:F:416:GLY:HA2	2.49	0.48
1:F:712:THR:HG23	1:F:714:LYS:H	1.79	0.48
1:C:366:TRP:HZ2	1:C:369:LEU:HD11	1.79	0.48
1:E:97:TYR:HE1	1:E:159:ASP:HB3	1.77	0.48
1:D:133:VAL:HG11	1:D:147:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:650:ARG:N	1:E:651:PRO:HD2	2.28	0.47
1:B:731:VAL:HG22	1:B:732:PHE:H	1.79	0.47
1:D:760:ILE:HD12	1:D:771:ASN:HB3	1.96	0.47
1:B:279:MET:HE2	1:B:279:MET:HA	1.97	0.47
1:E:124:ALA:HB2	1:E:162:ILE:HG12	1.95	0.47
1:A:665:TRP:HB3	1:A:667:LEU:HG	1.96	0.47
1:D:560:PRO:HA	1:D:680:LYS:HE2	1.96	0.47
1:D:643:VAL:HG21	1:D:690:HIS:HE1	1.79	0.47
1:F:789:VAL:O	1:F:790:LYS:HB2	2.15	0.47
1:A:86:TYR:OH	1:A:595:ARG:HG3	2.14	0.47
1:D:686:MET:HA	1:D:689:VAL:HG22	1.97	0.47
1:E:267:ARG:HD2	1:E:307:TYR:CE2	2.50	0.47
1:F:336:LEU:HD11	1:F:350:PHE:CD2	2.49	0.47
1:A:184:ASN:OD1	1:A:186:GLU:HG3	2.15	0.47
1:A:640:LYS:HG3	1:A:689:VAL:HG11	1.97	0.47
1:B:207:SER:OG	1:B:208:ALA:N	2.47	0.47
1:C:544:THR:HG23	1:C:545:GLU:HG3	1.96	0.47
1:C:559:CYS:H	1:C:631:SER:HB3	1.80	0.47
1:B:736:PHE:HZ	1:B:764:ILE:HD11	1.79	0.46
1:D:661:ILE:HG13	1:D:672:ILE:HD11	1.96	0.46
1:D:708:VAL:HB	1:D:746:ILE:HD11	1.97	0.46
1:F:736:PHE:HB2	1:F:746:ILE:HD12	1.97	0.46
1:A:639:MET:HA	1:A:639:MET:HE2	1.98	0.46
1:B:727:SER:N	1:B:791:LYS:HZ1	2.13	0.46
1:C:128:VAL:HG21	1:C:147:ILE:HG21	1.97	0.46
1:F:537:TYR:CE2	1:F:539:LYS:HB2	2.50	0.46
1:B:379:HIS:CG	1:B:662:ARG:NH2	2.84	0.46
1:C:362:LYS:HB2	1:C:690:HIS:HE1	1.78	0.46
1:C:594:ASN:HD21	1:C:667:LEU:HD13	1.80	0.46
1:D:244:SER:HB3	1:D:285:LEU:HD11	1.96	0.46
1:A:486:ARG:O	1:A:490:GLN:HB3	2.16	0.46
1:B:39:GLN:NE2	1:B:43:PRO:HB3	2.30	0.46
1:C:363:GLY:O	1:C:657:ILE:HA	2.15	0.46
1:C:650:ARG:O	1:C:652:TYR:N	2.49	0.46
1:C:686:MET:HA	1:C:689:VAL:HG22	1.97	0.46
1:E:639:MET:HB3	1:E:686:MET:SD	2.56	0.46
1:C:363:GLY:HA3	1:C:394:ILE:O	2.16	0.46
1:C:568:MET:HG2	1:C:666:PRO:HB3	1.98	0.46
1:E:336:LEU:HB2	1:E:504:PRO:HG3	1.98	0.46
1:F:541:PRO:HA	1:F:544:THR:HG22	1.97	0.46
1:F:595:ARG:HG3	1:F:601:PHE:HE1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:ALA:HB3	1:A:665:TRP:CZ3	2.51	0.45
1:D:563:GLU:HG2	3:D:805:EDO:H21	1.98	0.45
1:C:80:MET:HE3	1:C:375:ARG:HH22	1.82	0.45
1:F:301:TYR:CE1	1:F:359:VAL:HG13	2.51	0.45
1:B:565:LEU:HD22	1:B:569:PHE:HE2	1.82	0.45
1:A:314:VAL:HG22	1:A:321:ILE:HG12	1.98	0.45
1:B:632:GLN:HB3	1:B:681:GLN:HB2	1.98	0.45
1:C:124:ALA:HB2	1:C:162:ILE:HG12	1.97	0.45
1:D:661:ILE:HA	1:D:672:ILE:HG12	1.99	0.45
1:E:34:LEU:HD11	1:E:96:TRP:HB3	1.98	0.45
1:D:624:LEU:O	1:D:628:ILE:HG12	2.16	0.45
1:C:199:TRP:CD1	1:C:200:ASP:H	2.35	0.45
1:F:267:ARG:HG2	1:F:272:ILE:HD11	1.99	0.45
1:F:788:TRP:O	1:F:789:VAL:C	2.59	0.45
1:A:166:VAL:HG13	1:A:186:GLU:CD	2.42	0.45
1:A:361:ALA:HA	1:A:393:ASN:ND2	2.31	0.45
1:F:107:VAL:HG13	1:F:111:GLN:HB2	1.98	0.45
1:B:36:PHE:HZ	1:B:75:LEU:HD13	1.83	0.44
1:B:334:VAL:HG21	1:B:458:ILE:HB	1.99	0.44
1:C:140:LEU:HB3	1:C:403:TYR:HD2	1.82	0.44
1:E:575:ASN:OD1	1:E:576:PRO:HD2	2.17	0.44
1:F:203:PRO:HD3	1:F:667:LEU:HD11	1.99	0.44
1:F:279:MET:HA	1:F:279:MET:HE2	1.99	0.44
1:F:396:ARG:HA	1:F:420:TRP:HB3	2.00	0.44
1:C:660:ASN:HD21	1:C:663:ASP:HA	1.82	0.44
1:B:578:GLN:O	1:B:581:VAL:HG22	2.17	0.44
1:A:44:VAL:HB	1:A:95:GLN:HE22	1.83	0.44
1:A:591:THR:HG1	1:A:595:ARG:HH21	1.64	0.44
1:D:590:GLN:HB3	1:D:595:ARG:HH21	1.83	0.44
1:B:736:PHE:CZ	1:B:764:ILE:HD11	2.53	0.44
1:C:296:TRP:CZ2	1:C:416:GLY:HA2	2.53	0.44
1:D:134:GLY:HA3	1:D:145:TYR:CE1	2.53	0.44
1:F:658:TRP:CD1	1:F:658:TRP:H	2.34	0.44
1:D:440:LEU:HD21	1:D:492:LEU:HD21	1.99	0.44
1:E:279:MET:HE2	1:E:279:MET:HA	1.99	0.44
1:F:253:PHE:HA	1:F:256:HIS:ND1	2.33	0.44
1:D:576:PRO:HD3	1:D:624:LEU:HD13	2.00	0.44
1:F:267:ARG:HD2	1:F:307:TYR:CE2	2.53	0.44
1:B:122:THR:OG1	1:B:139:MET:HB2	2.18	0.43
1:D:247:LEU:CD2	1:D:249:THR:HG23	2.48	0.43
1:E:264:THR:HG23	1:E:310:GLU:HB3	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:GLU:HG2	1:B:88:LEU:HD13	2.00	0.43
1:E:44:VAL:HB	1:E:95:GLN:HE22	1.82	0.43
1:F:363:GLY:HA3	1:F:394:ILE:O	2.18	0.43
1:C:582:VAL:HB	1:C:620:VAL:HG21	1.99	0.43
1:C:334:VAL:HG21	1:C:458:ILE:HB	2.00	0.43
1:C:662:ARG:NH1	1:C:663:ASP:O	2.51	0.43
1:E:202:MET:HG3	1:E:203:PRO:HD2	2.00	0.43
1:E:306:LEU:HD21	1:E:413:ASP:HB3	2.00	0.43
1:B:179:ILE:HB	1:C:246:TYR:HD2	1.84	0.43
1:D:538:TYR:CE2	1:D:616:ILE:HD11	2.54	0.43
1:F:671:ALA:O	1:F:680:LYS:HE2	2.19	0.43
1:A:80:MET:HE2	1:A:676:TRP:HZ2	1.83	0.43
1:A:229:TRP:CZ2	1:A:309:ALA:HB1	2.53	0.43
1:C:708:VAL:HG12	1:C:746:ILE:HD11	2.01	0.43
1:D:98:TYR:HB2	1:D:160:VAL:HG13	2.01	0.43
1:A:92:GLU:HB2	1:B:253:PHE:CZ	2.53	0.43
1:A:426:GLY:O	1:A:427:CYS:C	2.62	0.43
1:A:679:LYS:HD3	1:A:683:PHE:CE2	2.53	0.43
1:B:263:ILE:HG21	1:B:288:LEU:HD11	2.01	0.43
1:F:199:TRP:CD1	1:F:200:ASP:H	2.35	0.43
1:F:414:LYS:HE3	1:F:415:TYR:CZ	2.54	0.43
1:C:191:ARG:HA	1:C:191:ARG:NH1	2.34	0.43
1:E:739:LYS:HA	1:E:739:LYS:HD2	1.76	0.43
1:E:128:VAL:HG12	1:E:129:ASN:ND2	2.34	0.43
1:B:179:ILE:HD11	1:C:248:GLN:HE21	1.84	0.42
1:E:193:ALA:HB3	1:E:196:THR:HG23	2.01	0.42
1:E:222:VAL:HG22	1:E:252:PRO:HD2	2.01	0.42
1:F:358:PRO:HG2	1:F:741:ASN:HD21	1.84	0.42
1:F:565:LEU:HD23	1:F:624:LEU:HD21	2.01	0.42
1:F:774:LEU:HD21	1:F:780:TYR:CE2	2.54	0.42
1:B:138:ASN:HD21	1:B:443:GLU:HB2	1.84	0.42
1:A:191:ARG:HD3	1:A:443:GLU:OE1	2.19	0.42
1:D:486:ARG:O	1:D:490:GLN:HB3	2.19	0.42
1:D:203:PRO:HD3	1:D:667:LEU:HD11	2.00	0.42
1:F:349:GLN:HG3	1:F:549:GLN:H	1.84	0.42
1:D:556:TYR:HE2	1:D:634:VAL:HG22	1.85	0.42
1:F:362:LYS:HB2	1:F:690:HIS:CE1	2.54	0.42
1:A:306:LEU:HD21	1:A:413:ASP:HB3	2.01	0.42
1:A:363:GLY:HA2	1:A:392:CYS:HB3	2.01	0.42
1:A:797:LEU:HD23	1:A:797:LEU:HA	1.89	0.42
1:C:201:ILE:HG21	1:C:660:ASN:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:ALA:O	1:D:276:GLU:HA	2.20	0.42
1:D:496:ILE:HG21	1:D:505:TYR:HB2	2.02	0.42
1:D:586:ASN:HD21	1:D:589:TRP:CD1	2.38	0.42
1:E:366:TRP:HZ2	1:E:369:LEU:HD11	1.85	0.42
1:E:586:ASN:HD21	1:E:589:TRP:CD1	2.38	0.42
1:F:366:TRP:HZ2	1:F:369:LEU:HD11	1.83	0.42
1:F:557:HIS:O	1:F:635:GLN:HB2	2.20	0.42
1:F:595:ARG:HG3	1:F:601:PHE:CE1	2.55	0.42
1:F:610:THR:C	1:F:612:GLN:N	2.78	0.42
1:F:787:LYS:HG3	1:F:788:TRP:N	2.34	0.42
1:A:336:LEU:HD11	1:A:350:PHE:CD1	2.54	0.42
1:B:40:PRO:HG2	1:B:44:VAL:HG23	2.00	0.42
1:C:267:ARG:O	1:C:270:ARG:HG2	2.19	0.42
1:B:577:TRP:HB3	1:B:581:VAL:O	2.19	0.42
1:A:491:VAL:O	1:A:495:VAL:HG23	2.19	0.42
1:A:537:TYR:CE2	1:A:539:LYS:HB2	2.55	0.42
1:C:253:PHE:HA	1:C:256:HIS:ND1	2.35	0.42
1:C:646:TRP:CD1	1:C:653:ARG:HB3	2.54	0.42
1:D:336:LEU:HD11	1:D:350:PHE:CD1	2.54	0.42
1:D:718:GLY:HA3	1:D:763:ARG:O	2.19	0.42
1:E:201:ILE:HD13	1:E:659:TRP:CZ2	2.54	0.42
1:E:203:PRO:HA	1:E:594:ASN:CG	2.45	0.42
1:E:556:TYR:HE2	1:E:634:VAL:HG12	1.84	0.42
1:F:660:ASN:CG	1:F:671:ALA:HB2	2.45	0.42
1:B:42:VAL:O	1:B:42:VAL:CG1	2.68	0.42
1:B:251:LEU:HD22	1:B:256:HIS:CD2	2.55	0.42
1:C:134:GLY:HA3	1:C:145:TYR:CE1	2.54	0.42
1:C:564:THR:O	1:C:568:MET:HG3	2.20	0.42
1:D:743:MET:HE3	1:D:743:MET:HB3	1.79	0.42
1:B:790:LYS:HG3	1:B:797:LEU:HD21	2.02	0.41
1:A:39:GLN:HB2	1:A:95:GLN:HG3	2.00	0.41
1:B:97:TYR:HE1	1:B:159:ASP:HB3	1.86	0.41
1:D:207:SER:OG	1:D:208:ALA:N	2.53	0.41
1:E:86:TYR:OH	1:E:595:ARG:HB3	2.20	0.41
1:A:591:THR:OG1	1:A:595:ARG:NH2	2.48	0.41
1:D:39:GLN:HB2	1:D:95:GLN:HG3	2.03	0.41
1:D:568:MET:HE3	1:D:569:PHE:CE2	2.55	0.41
1:A:429:ASN:OD1	1:A:429:ASN:N	2.52	0.41
1:A:456:SER:O	1:A:458:ILE:HG23	2.20	0.41
1:A:458:ILE:O	1:A:504:PRO:HD2	2.20	0.41
1:A:661:ILE:HA	1:A:672:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:ARG:NH1	1:F:191:ARG:HA	2.35	0.41
1:F:661:ILE:HG13	1:F:672:ILE:HD11	2.02	0.41
1:B:551:VAL:HG23	1:B:656:ILE:HA	2.02	0.41
1:C:689:VAL:HA	1:C:694:CYS:SG	2.61	0.41
1:A:366:TRP:CZ2	1:A:369:LEU:HD21	2.56	0.41
1:A:420:TRP:CD1	1:A:420:TRP:C	2.99	0.41
1:B:643:VAL:HG21	1:B:690:HIS:HE1	1.85	0.41
1:E:420:TRP:CD1	1:E:420:TRP:C	2.99	0.41
1:E:591:THR:HG1	1:E:595:ARG:HH21	1.68	0.41
1:A:587:ASP:OD1	1:A:595:ARG:NH2	2.54	0.41
1:D:306:LEU:HD21	1:D:413:ASP:HB3	2.02	0.41
1:E:230:VAL:HG13	1:E:502:THR:HG21	2.02	0.41
1:A:199:TRP:CD1	1:A:200:ASP:H	2.39	0.41
1:A:253:PHE:HA	1:A:256:HIS:ND1	2.36	0.41
1:A:362:LYS:H	1:A:393:ASN:CG	2.27	0.41
1:B:211:TRP:H	1:B:211:TRP:CD1	2.38	0.41
1:C:665:TRP:CG	1:C:666:PRO:HD2	2.56	0.41
1:D:565:LEU:HD11	1:D:628:ILE:HD11	2.01	0.41
1:E:244:SER:HB3	1:E:285:LEU:HD11	2.02	0.41
1:E:661:ILE:HA	1:E:672:ILE:HG12	2.03	0.41
1:F:244:SER:HB3	1:F:285:LEU:HD11	2.02	0.41
1:F:366:TRP:HB3	1:F:397:CYS:HA	2.03	0.41
1:F:391:ASN:HB3	1:F:690:HIS:O	2.21	0.41
1:F:576:PRO:HD3	1:F:624:LEU:HD13	2.02	0.41
1:A:279:MET:HE2	1:A:279:MET:HA	2.03	0.41
1:E:192:ARG:HD3	1:E:197:TYR:OH	2.20	0.41
1:A:334:VAL:HG21	1:A:458:ILE:HB	2.03	0.40
1:A:363:GLY:HA3	1:A:394:ILE:O	2.21	0.40
1:C:298:PRO:HD3	1:C:354:ILE:HG21	2.03	0.40
1:A:698:ASN:HD22	1:A:698:ASN:HA	1.73	0.40
1:B:205:LEU:O	1:B:206:VAL:C	2.64	0.40
1:B:592:LYS:HD3	1:B:592:LYS:HA	1.91	0.40
1:C:710:ASN:ND2	1:C:740:ALA:HA	2.36	0.40
1:D:595:ARG:O	1:D:596:ILE:C	2.64	0.40
1:D:762:TYR:CE2	1:D:769:TYR:HB2	2.55	0.40
1:E:576:PRO:HD3	1:E:624:LEU:HD13	2.03	0.40
1:F:650:ARG:N	1:F:651:PRO:HD2	2.36	0.40
1:F:791:LYS:O	1:F:792:CYS:C	2.65	0.40
1:B:660:ASN:HB3	1:B:671:ALA:CB	2.51	0.40
1:E:27:SER:HA	1:E:215:THR:HG22	2.03	0.40
1:F:647:ARG:NH2	1:F:709:ASP:HB3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLN:HG2	1:A:163:ARG:HA	2.02	0.40
1:A:786:ARG:HG3	1:A:797:LEU:HD13	2.03	0.40
1:B:660:ASN:HB3	1:B:671:ALA:CA	2.50	0.40
1:B:736:PHE:HZ	1:B:764:ILE:CD1	2.33	0.40
1:C:195:SER:C	1:C:197:TYR:H	2.29	0.40
1:D:34:LEU:HD11	1:D:96:TRP:HB3	2.03	0.40
1:E:280:ARG:HD3	1:F:597:TYR:HB3	2.04	0.40
1:F:34:LEU:HB2	1:F:60:ALA:HB2	2.03	0.40
1:F:643:VAL:HA	1:F:656:ILE:HD13	2.03	0.40
1:B:576:PRO:HB3	1:B:589:TRP:CH2	2.56	0.40
1:B:743:MET:HE3	1:B:743:MET:HB3	2.01	0.40
1:E:457:LEU:HD22	1:E:503:ARG:HD3	2.03	0.40
1:F:70:MET:HE3	1:F:96:TRP:HZ3	1.87	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	718/798 (90%)	679 (95%)	37 (5%)	2 (0%)	36	67
1	B	717/798 (90%)	692 (96%)	25 (4%)	0	100	100
1	C	706/798 (88%)	667 (94%)	37 (5%)	2 (0%)	36	67
1	D	705/798 (88%)	675 (96%)	29 (4%)	1 (0%)	48	78
1	E	718/798 (90%)	682 (95%)	34 (5%)	2 (0%)	36	67
1	F	678/798 (85%)	629 (93%)	42 (6%)	7 (1%)	12	41
All	All	4242/4788 (89%)	4024 (95%)	204 (5%)	14 (0%)	36	67

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	594	ASN
1	F	610	THR
1	F	666	PRO
1	F	299	ARG
1	C	666	PRO
1	D	594	ASN
1	F	660	ASN
1	A	598	ASP
1	C	660	ASN
1	A	666	PRO
1	F	788	TRP
1	F	790	LYS
1	F	667	LEU
1	E	746	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	626/688 (91%)	623 (100%)	3 (0%)	81	85
1	B	625/688 (91%)	622 (100%)	3 (0%)	81	85
1	C	623/688 (91%)	618 (99%)	5 (1%)	73	81
1	D	618/688 (90%)	615 (100%)	3 (0%)	81	85
1	E	626/688 (91%)	625 (100%)	1 (0%)	87	89
1	F	607/688 (88%)	601 (99%)	6 (1%)	68	79
All	All	3725/4128 (90%)	3704 (99%)	21 (1%)	78	83

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	ILE
1	A	487	VAL
1	A	792	CYS
1	B	44	VAL
1	B	341	VAL

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Mol	Chain	Res	Type
1	B	594	ASN
1	C	201	ILE
1	C	205	LEU
1	C	620	VAL
1	C	660	ASN
1	C	794	ILE
1	D	205	LEU
1	D	602	GLN
1	D	745	GLU
1	E	591	THR
1	F	656	ILE
1	F	658	TRP
1	F	725	VAL
1	F	755	GLN
1	F	787	LYS
1	F	789	VAL

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

Mol	Chain	Res	Type
1	A	349	GLN
1	A	407	HIS
1	A	454	HIS
1	A	549	GLN
1	A	575	ASN
1	B	373	HIS
1	B	421	GLN
1	B	546	ASN
1	B	602	GLN
1	B	681	GLN
1	C	170	GLN
1	C	228	ASN
1	C	575	ASN
1	C	752	GLN
1	D	228	ASN
1	D	284	ASN
1	D	342	ASN
1	D	421	GLN
1	D	575	ASN
1	D	594	ASN
1	D	612	GLN
1	D	660	ASN

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Mol	Chain	Res	Type
1	D	767	ASN
1	E	129	ASN
1	E	172	HIS
1	E	385	GLN
1	E	611	ASN
1	E	660	ASN
1	E	681	GLN
1	F	612	GLN
1	F	711	ASN
1	F	742	GLN
1	F	755	GLN
1	F	784	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

32 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	F	802	-	4,4,4	1.60	1 (25%)	6,6,6	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	D	804	-	4,4,4	1.59	1 (25%)	6,6,6	0.47	0
2	PO4	F	801	-	4,4,4	1.57	1 (25%)	6,6,6	0.50	0
2	PO4	F	803	-	4,4,4	1.60	1 (25%)	6,6,6	0.47	0
2	PO4	C	803	-	4,4,4	1.60	1 (25%)	6,6,6	0.50	0
3	EDO	F	805	-	3,3,3	0.09	0	2,2,2	0.07	0
3	EDO	A	804	-	3,3,3	0.11	0	2,2,2	0.14	0
2	PO4	C	802	-	4,4,4	1.59	1 (25%)	6,6,6	0.45	0
2	PO4	E	801	-	4,4,4	1.54	1 (25%)	6,6,6	0.51	0
2	PO4	D	802	-	4,4,4	1.58	1 (25%)	6,6,6	0.50	0
2	PO4	C	804	-	4,4,4	1.58	1 (25%)	6,6,6	0.48	0
2	PO4	B	802	-	4,4,4	1.59	1 (25%)	6,6,6	0.48	0
2	PO4	A	802	-	4,4,4	1.59	1 (25%)	6,6,6	0.48	0
3	EDO	F	804	-	3,3,3	0.25	0	2,2,2	0.28	0
2	PO4	C	801	-	4,4,4	1.58	1 (25%)	6,6,6	0.52	0
3	EDO	A	805	-	3,3,3	0.10	0	2,2,2	0.07	0
3	EDO	E	806	-	3,3,3	0.10	0	2,2,2	0.05	0
2	PO4	E	802	-	4,4,4	1.57	1 (25%)	6,6,6	0.47	0
2	PO4	A	801	-	4,4,4	1.57	1 (25%)	6,6,6	0.50	0
2	PO4	B	801	-	4,4,4	1.58	1 (25%)	6,6,6	0.46	0
2	PO4	E	804	-	4,4,4	0.74	0	6,6,6	0.46	0
2	PO4	C	806	-	4,4,4	1.59	1 (25%)	6,6,6	0.50	0
3	EDO	E	807	-	3,3,3	0.09	0	2,2,2	0.14	0
2	PO4	D	801	-	4,4,4	1.55	1 (25%)	6,6,6	0.56	0
2	PO4	A	803	-	4,4,4	1.57	1 (25%)	6,6,6	0.52	0
2	PO4	D	803	-	4,4,4	1.60	1 (25%)	6,6,6	0.50	0
2	PO4	C	805	-	4,4,4	1.57	1 (25%)	6,6,6	0.49	0
3	EDO	D	805	-	3,3,3	0.07	0	2,2,2	0.14	0
3	EDO	C	807	-	3,3,3	0.08	0	2,2,2	0.09	0
3	EDO	E	805	-	3,3,3	0.25	0	2,2,2	0.29	0
3	EDO	B	803	-	3,3,3	0.06	0	2,2,2	0.13	0
2	PO4	E	803	-	4,4,4	1.56	1 (25%)	6,6,6	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	E	807	-	-	1/1/1/1	-
3	EDO	F	804	-	-	0/1/1/1	-
3	EDO	A	805	-	-	0/1/1/1	-
3	EDO	E	806	-	-	1/1/1/1	-
3	EDO	D	805	-	-	0/1/1/1	-
3	EDO	C	807	-	-	1/1/1/1	-
3	EDO	A	804	-	-	0/1/1/1	-
3	EDO	E	805	-	-	0/1/1/1	-
3	EDO	B	803	-	-	1/1/1/1	-
3	EDO	F	805	-	-	0/1/1/1	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	802	PO4	P-O1	2.79	1.57	1.50
2	A	802	PO4	P-O1	2.78	1.57	1.50
2	C	806	PO4	P-O1	2.77	1.57	1.50
2	F	803	PO4	P-O1	2.77	1.57	1.50
2	C	802	PO4	P-O1	2.77	1.57	1.50
2	D	803	PO4	P-O1	2.77	1.57	1.50
2	C	803	PO4	P-O1	2.76	1.57	1.50
2	D	804	PO4	P-O1	2.75	1.57	1.50
2	B	802	PO4	P-O1	2.75	1.57	1.50
2	A	801	PO4	P-O1	2.74	1.57	1.50
2	B	801	PO4	P-O1	2.74	1.57	1.50
2	C	801	PO4	P-O1	2.74	1.57	1.50
2	D	802	PO4	P-O1	2.73	1.57	1.50
2	C	804	PO4	P-O1	2.72	1.56	1.50
2	C	805	PO4	P-O1	2.72	1.56	1.50
2	F	801	PO4	P-O1	2.72	1.56	1.50
2	E	802	PO4	P-O1	2.71	1.56	1.50
2	E	803	PO4	P-O1	2.69	1.56	1.50
2	A	803	PO4	P-O1	2.69	1.56	1.50
2	E	801	PO4	P-O1	2.68	1.56	1.50
2	D	801	PO4	P-O1	2.68	1.56	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	803	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	C	807	EDO	O1-C1-C2-O2
3	E	806	EDO	O1-C1-C2-O2
3	E	807	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	805	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	726/798 (90%)	0.19	4 (0%)	85 70	44, 69, 101, 149	0
1	B	725/798 (90%)	0.26	29 (4%)	42 23	44, 79, 134, 169	0
1	C	718/798 (89%)	0.45	35 (4%)	35 18	44, 80, 139, 198	0
1	D	717/798 (89%)	0.24	15 (2%)	63 42	41, 74, 124, 163	0
1	E	726/798 (90%)	0.36	13 (1%)	67 47	47, 78, 117, 168	0
1	F	700/798 (87%)	0.59	48 (6%)	23 12	48, 94, 143, 178	0
All	All	4312/4788 (90%)	0.35	144 (3%)	49 29	41, 78, 133, 198	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	392	CYS	5.7
1	F	556	TYR	5.0
1	C	594	ASN	4.9
1	F	538	TYR	4.6
1	B	659	TRP	4.5
1	D	703	GLY	4.3
1	F	201	ILE	4.1
1	C	617	PHE	3.9
1	E	594	ASN	3.7
1	B	732	PHE	3.7
1	C	465	ALA	3.6
1	B	731	VAL	3.5
1	C	685	TYR	3.4
1	F	426	GLY	3.4
1	F	612	GLN	3.4
1	F	761	SER	3.4
1	C	361	ALA	3.4
1	E	321	ILE	3.3
1	B	730	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	792	CYS	3.3
1	E	463	ASN	3.2
1	F	594	ASN	3.2
1	D	749	LEU	3.2
1	F	613	VAL	3.2
1	F	720	VAL	3.2
1	F	630	ALA	3.2
1	C	426	GLY	3.2
1	F	536	GLY	3.2
1	F	760	ILE	3.2
1	B	358	PRO	3.1
1	F	793	GLY	3.1
1	E	531	LEU	3.0
1	C	201	ILE	3.0
1	D	536	GLY	3.0
1	C	482	PRO	2.9
1	B	583	GLY	2.9
1	F	756	GLY	2.9
1	B	760	ILE	2.9
1	C	538	TYR	2.9
1	B	738	SER	2.9
1	F	795	TYR	2.9
1	F	693	VAL	2.8
1	F	609	MET	2.8
1	A	697	ILE	2.8
1	B	463	ASN	2.8
1	C	558	GLY	2.8
1	C	463	ASN	2.7
1	C	548	SER	2.7
1	C	556	TYR	2.7
1	D	750	PRO	2.7
1	D	340	GLU	2.7
1	B	733	LYS	2.7
1	C	582	VAL	2.7
1	C	621	PRO	2.7
1	D	508	SER	2.7
1	F	631	SER	2.7
1	C	630	ALA	2.6
1	F	673	SER	2.6
1	A	47	ILE	2.6
1	C	663	ASP	2.6
1	F	621	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	536	GLY	2.6
1	B	633	SER	2.6
1	B	534	PRO	2.6
1	B	787	LYS	2.6
1	E	534	PRO	2.6
1	F	670	ASP	2.6
1	A	688	ASN	2.6
1	F	685	TYR	2.5
1	F	771	ASN	2.5
1	C	682	ALA	2.5
1	C	659	TRP	2.5
1	F	696	LEU	2.5
1	F	620	VAL	2.5
1	B	734	GLY	2.4
1	D	23	VAL	2.4
1	B	508	SER	2.4
1	E	422	ASP	2.4
1	B	728	GLY	2.4
1	D	725	VAL	2.4
1	B	797	LEU	2.4
1	F	392	CYS	2.4
1	F	672	ILE	2.4
1	F	348	GLY	2.4
1	F	663	ASP	2.4
1	E	155	GLU	2.4
1	B	737	VAL	2.4
1	C	348	GLY	2.3
1	F	555	GLY	2.3
1	C	616	ILE	2.3
1	F	597	TYR	2.3
1	C	620	VAL	2.3
1	B	729	LYS	2.3
1	F	361	ALA	2.3
1	B	743	MET	2.3
1	B	759	VAL	2.3
1	F	785	TYR	2.3
1	F	789	VAL	2.3
1	A	669	SER	2.3
1	F	481	ASN	2.3
1	F	725	VAL	2.3
1	F	779	PRO	2.3
1	B	727	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	656	ILE	2.2
1	C	688	ASN	2.2
1	B	356	GLY	2.2
1	F	667	LEU	2.2
1	C	660	ASN	2.2
1	F	695	CYS	2.2
1	E	236	PRO	2.2
1	F	773	TYR	2.2
1	C	613	VAL	2.2
1	C	596	ILE	2.2
1	E	568	MET	2.2
1	C	583	GLY	2.2
1	F	690	HIS	2.2
1	B	300	GLY	2.2
1	C	555	GLY	2.2
1	D	736	PHE	2.2
1	B	359	VAL	2.1
1	C	667	LEU	2.1
1	C	771	ASN	2.1
1	E	347	PRO	2.1
1	C	673	SER	2.1
1	F	389	GLU	2.1
1	F	618	GLY	2.1
1	F	796	GLU	2.1
1	B	641	PHE	2.1
1	D	724	ASP	2.1
1	D	668	LEU	2.1
1	D	729	LYS	2.1
1	D	730	GLN	2.1
1	D	557	HIS	2.1
1	F	788	TRP	2.1
1	D	356	GLY	2.1
1	C	668	LEU	2.1
1	C	686	MET	2.1
1	F	622	ALA	2.1
1	F	634	VAL	2.0
1	E	669	SER	2.0
1	E	177	LEU	2.0
1	B	557	HIS	2.0
1	B	757	MET	2.0
1	C	726	ALA	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
2	PO4	C	804	5/5	0.49	0.18	103,119,124,126	0
2	PO4	C	805	5/5	0.51	0.21	102,122,123,129	0
3	EDO	F	805	4/4	0.52	0.28	66,70,75,78	0
2	PO4	C	806	5/5	0.54	0.23	97,105,144,146	0
2	PO4	D	804	5/5	0.58	0.17	95,100,108,122	0
2	PO4	C	803	5/5	0.61	0.20	90,93,106,131	0
2	PO4	E	803	5/5	0.64	0.13	117,124,135,139	0
2	PO4	F	803	5/5	0.65	0.21	81,88,101,116	0
3	EDO	E	805	4/4	0.65	0.15	65,67,75,77	0
3	EDO	F	804	4/4	0.65	0.21	79,80,81,84	0
2	PO4	E	804	5/5	0.65	0.24	102,114,139,147	0
2	PO4	E	802	5/5	0.66	0.17	108,112,117,128	0
2	PO4	C	802	5/5	0.67	0.24	81,92,121,132	0
2	PO4	D	802	5/5	0.71	0.10	80,87,97,110	0
2	PO4	A	803	5/5	0.75	0.23	83,92,95,118	0
3	EDO	C	807	4/4	0.76	0.30	59,62,65,65	0
2	PO4	D	803	5/5	0.77	0.19	72,85,99,134	0
3	EDO	A	804	4/4	0.78	0.16	40,53,54,58	0
3	EDO	B	803	4/4	0.80	0.20	79,94,101,105	0
2	PO4	B	802	5/5	0.81	0.10	75,80,90,101	0
2	PO4	A	802	5/5	0.83	0.16	79,81,92,100	0
2	PO4	E	801	5/5	0.83	0.10	66,75,86,99	0
3	EDO	E	806	4/4	0.86	0.17	66,68,72,73	0
3	EDO	E	807	4/4	0.86	0.16	50,53,56,57	0
3	EDO	D	805	4/4	0.87	0.22	74,81,84,87	0
2	PO4	C	801	5/5	0.88	0.10	50,54,71,87	0
2	PO4	F	802	5/5	0.88	0.15	79,83,111,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	F	801	5/5	0.91	0.09	66,66,76,97	0
2	PO4	D	801	5/5	0.92	0.09	52,69,74,76	0
3	EDO	A	805	4/4	0.92	0.14	63,68,70,70	0
2	PO4	B	801	5/5	0.93	0.08	56,65,74,85	0
2	PO4	A	801	5/5	0.94	0.09	60,60,71,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.