



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:37 PM UTC

PDB ID : 1ZZ8 / pdb_00001zz8
Title : Crystal Structure of FeII HppE in Complex with Substrate Form 2
Authors : Higgins, L.J.; Yan, F.; Liu, P.; Liu, H.W.; Drennan, C.L.
Deposited on : 2005-06-13
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

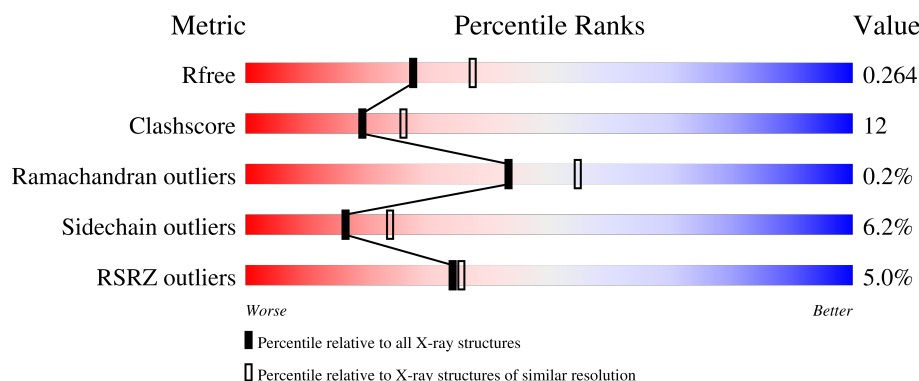
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	198	5% 74% 20% • •
1	B	198	7% 68% 24% 5% •
1	C	198	3% 68% 24% • • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4515 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.

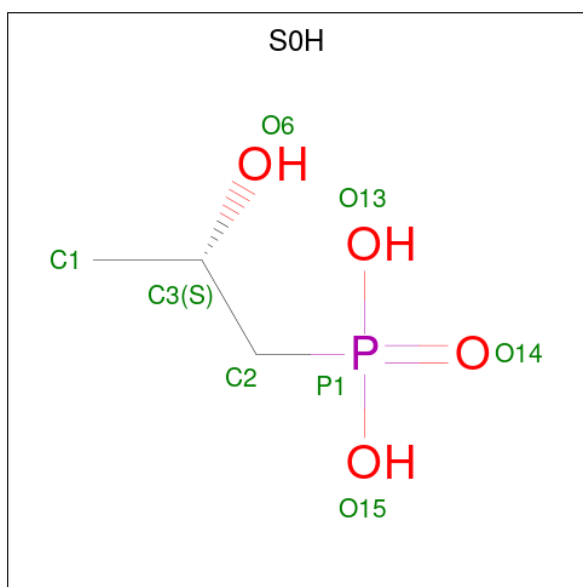
- Molecule 1 is a protein called Hydroxypropylphosphonic Acid Epoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1445	914	246	280	5			
1	B	193	Total	C	N	O	S	0	0	0
			1451	918	250	278	5			
1	C	192	Total	C	N	O	S	0	0	0
			1446	914	248	279	5			

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		

- Molecule 3 is (S)-2-HYDROXYPROPYLPHOSPHONIC ACID (CCD ID: S0H) (formula: C₃H₉O₄P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			8	3	4	1		
3	B	1	Total	C	O	P	0	0
			8	3	4	1		
3	C	1	Total	C	O	P	0	0
			8	3	4	1		

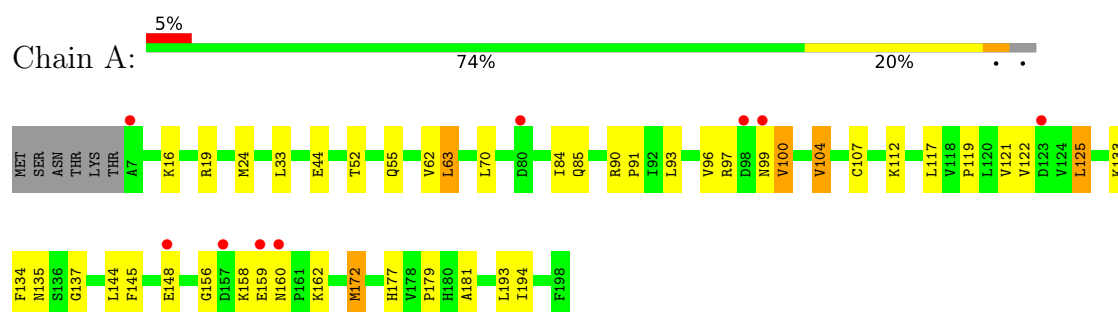
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total	O	0	0
			51	51		
4	B	31	Total	O	0	0
			31	31		
4	C	64	Total	O	0	0
			64	64		

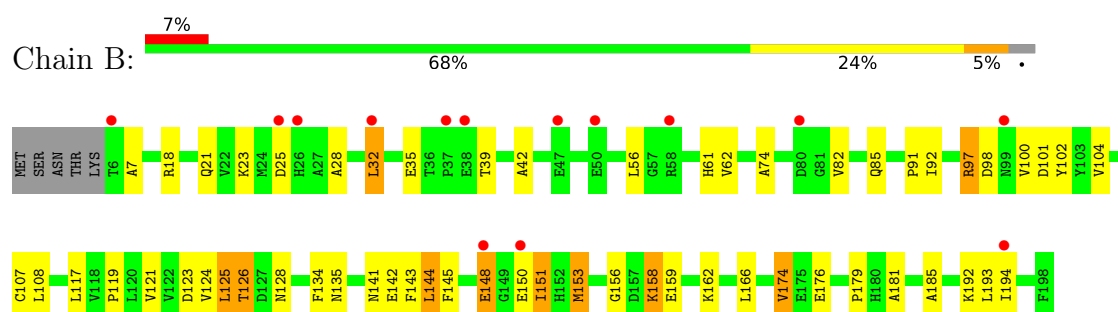
3 Residue-property plots [i](#)

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.

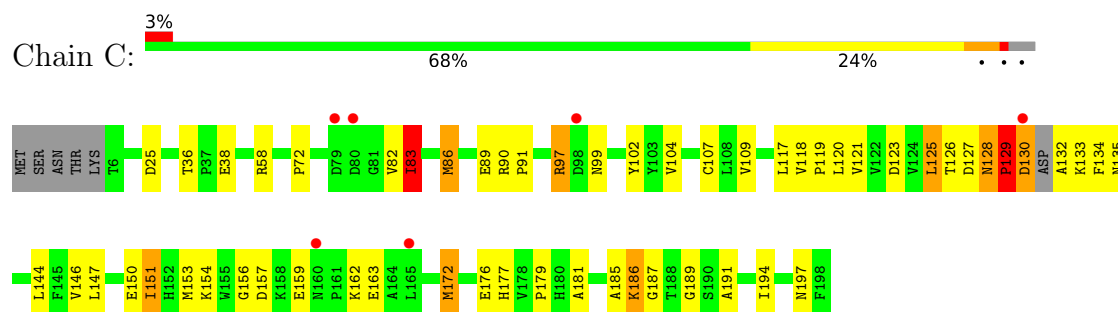
• Molecule 1: Hydroxypropylphosphonic Acid Epoxidase



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4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	111.65Å 111.65Å 152.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.3 (30.00-2.30) 96.3 (30.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.84 (at 2.31Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.225 , 0.252 0.237 , 0.264	Depositor DCC
R_{free} test set	1852 reflections (4.31%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtrriage
Anisotropy	0.133	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4515	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1656e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: S0H, FE2

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	0.50	0/1475	1.02	6/2007 (0.3%)
1	B	0.55	1/1481 (0.1%)	1.08	10/2015 (0.5%)
1	C	0.59	3/1475 (0.2%)	1.10	13/2006 (0.6%)
All	All	0.55	4/4431 (0.1%)	1.07	29/6028 (0.5%)

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	C	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	153	MET	SD-CE	-8.59	1.58	1.79
1	C	86	MET	SD-CE	-8.08	1.59	1.79
1	C	83	ILE	C-O	5.64	1.29	1.24
1	C	153	MET	SD-CE	-5.05	1.67	1.79

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	ASN	N-CA-C	-8.66	97.48	109.95
1	B	7	ALA	N-CA-C	-8.61	101.86	111.07
1	C	194	ILE	N-CA-C	-8.55	95.40	107.80
1	A	135	ASN	N-CA-C	-7.89	97.49	109.96
1	C	135	ASN	N-CA-C	-7.82	98.36	110.17
1	A	162	LYS	N-CA-C	-7.73	99.08	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	VAL	N-CA-C	-7.33	97.57	108.12
1	C	90	ARG	CA-C-N	-6.99	112.77	119.76
1	C	90	ARG	C-N-CA	-6.99	112.77	119.76
1	C	121	VAL	N-CA-C	-6.99	97.02	107.37
1	C	162	LYS	N-CA-C	-6.94	101.18	110.55
1	B	121	VAL	N-CA-C	-6.89	97.81	107.80
1	C	109	VAL	N-CA-C	6.67	119.24	109.63
1	B	125	LEU	N-CA-C	6.63	118.59	111.36
1	A	99	ASN	N-CA-C	6.54	121.20	113.23
1	A	121	VAL	N-CA-C	-6.39	98.53	107.80
1	C	99	ASN	N-CA-CB	-6.27	107.02	114.17
1	B	74	ALA	N-CA-C	6.08	118.68	111.33
1	A	125	LEU	N-CA-C	6.08	119.16	111.69
1	B	151	ILE	N-CA-C	5.59	116.64	108.53
1	B	162	LYS	N-CA-C	-5.51	103.11	110.55
1	C	72	PRO	N-CA-C	5.50	117.41	110.70
1	C	25	ASP	N-CA-C	-5.45	101.94	110.17
1	B	56	LEU	N-CA-C	-5.25	105.64	111.36
1	B	25	ASP	N-CA-C	-5.17	102.51	109.95
1	C	128	ASN	CA-C-N	5.16	126.28	119.84
1	C	128	ASN	C-N-CA	5.16	126.28	119.84
1	C	125	LEU	N-CA-C	5.11	118.67	112.23
1	B	92	ILE	N-CA-C	5.10	115.46	108.12

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	83	ILE	Mainchain

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	1445	0	1420	27	0
1	B	1451	0	1426	43	0
1	C	1446	0	1422	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	8	0	3	0	0
3	B	8	0	3	0	0
3	C	8	0	3	0	0
4	A	51	0	0	0	1
4	B	31	0	0	5	0
4	C	64	0	0	0	0
All	All	4515	0	4277	101	1

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 12.

All (101) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:PRO:HG2	1:A:107:CYS:HB2	1.50	0.92
1:B:158:LYS:HD2	1:B:158:LYS:H	1.36	0.90
1:B:153:MET:HE2	1:B:166:LEU:HD11	1.53	0.88
1:B:145:PHE:HB3	1:B:194:ILE:HG22	1.58	0.85
1:A:145:PHE:HB3	1:A:194:ILE:HG22	1.62	0.80
1:C:186:LYS:HE3	1:C:187:GLY:N	1.97	0.78
1:B:145:PHE:HB3	1:B:194:ILE:CG2	2.15	0.76
1:B:91:PRO:HG2	1:B:107:CYS:HB2	1.66	0.76
1:C:146:VAL:HG13	1:C:151:ILE:HD13	1.66	0.76
1:B:148:GLU:OE1	1:B:192:LYS:HD3	1.87	0.74
1:C:154:LYS:HG2	1:C:163:GLU:HG2	1.68	0.74
1:B:126:THR:HG22	4:B:1007:HOH:O	1.92	0.70
1:A:145:PHE:HB3	1:A:194:ILE:CG2	2.24	0.68
1:B:102:TYR:CE1	1:B:126:THR:HG21	2.30	0.67
1:C:156:GLY:O	1:C:179:PRO:HG2	1.95	0.66
1:B:158:LYS:HD2	1:B:158:LYS:N	2.10	0.66
1:A:122:VAL:HB	1:A:193:LEU:CD1	2.26	0.66
1:C:144:LEU:HB2	1:C:172:MET:HG2	1.78	0.65
1:B:134:PHE:HA	1:B:181:ALA:HB2	1.81	0.63
1:B:153:MET:CE	1:B:166:LEU:HD11	2.27	0.62
1:B:32:LEU:HD22	1:B:62:VAL:HG13	1.83	0.61
1:C:104:VAL:HB	1:C:123:ASP:HB2	1.83	0.61
1:B:148:GLU:HG3	1:B:192:LYS:HB3	1.83	0.60
1:A:122:VAL:HB	1:A:193:LEU:HD11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:PRO:HG2	1:C:107:CYS:HB2	1.84	0.59
1:A:100:VAL:HG11	1:A:133:LYS:HZ2	1.68	0.59
1:A:144:LEU:HB2	1:A:172:MET:HG2	1.85	0.58
1:A:193:LEU:HD12	1:A:193:LEU:O	2.03	0.58
1:C:186:LYS:HE3	1:C:187:GLY:H	1.69	0.57
1:C:130:ASP:C	1:C:132:ALA:N	2.62	0.57
1:B:126:THR:CG2	4:B:1007:HOH:O	2.51	0.57
1:B:156:GLY:O	1:B:179:PRO:HG2	2.05	0.56
1:A:90:ARG:HB2	1:A:107:CYS:O	2.05	0.55
1:B:104:VAL:HG23	1:B:125:LEU:HD11	1.89	0.55
1:A:100:VAL:HG11	1:A:133:LYS:NZ	2.23	0.54
1:C:157:ASP:OD2	1:C:159:GLU:HB2	2.08	0.54
1:B:193:LEU:C	1:B:193:LEU:HD12	2.33	0.54
1:C:97:ARG:HG2	1:C:133:LYS:CB	2.38	0.53
1:C:97:ARG:HB2	1:C:102:TYR:HB2	1.91	0.52
1:B:23:LYS:HD2	1:B:23:LYS:N	2.23	0.52
1:C:150:GLU:HG2	1:C:185:ALA:HB2	1.91	0.52
1:C:58:ARG:HG2	1:C:58:ARG:HH11	1.74	0.52
1:C:151:ILE:HD11	1:C:191:ALA:HB1	1.92	0.52
1:C:107:CYS:HA	1:C:120:LEU:HD23	1.92	0.51
1:A:112:LYS:NZ	1:B:61:HIS:ND1	2.50	0.51
1:A:52:THR:OG1	1:A:55:GLN:HG3	2.11	0.51
1:B:142:GLU:HG2	1:B:144:LEU:HD22	1.93	0.51
1:A:117:LEU:HG	1:A:119:PRO:HD3	1.92	0.51
1:C:126:THR:HG22	1:C:128:ASN:H	1.74	0.51
1:C:146:VAL:HG13	1:C:151:ILE:CD1	2.39	0.51
1:B:141:ASN:ND2	1:B:176:GLU:H	2.09	0.50
1:B:128:ASN:C	1:B:128:ASN:HD22	2.18	0.50
1:A:134:PHE:HA	1:A:181:ALA:HB2	1.92	0.50
1:B:150:GLU:HB3	1:B:185:ALA:HB2	1.94	0.50
1:A:193:LEU:HD12	1:A:193:LEU:C	2.37	0.49
1:C:117:LEU:HG	1:C:119:PRO:HD3	1.94	0.49
1:B:18:ARG:HA	1:B:21:GLN:HE21	1.77	0.49
1:B:35:GLU:OE2	1:B:39:THR:HG21	2.12	0.49
1:B:39:THR:O	1:B:42:ALA:HB3	2.12	0.49
1:C:134:PHE:HA	1:C:181:ALA:HB2	1.95	0.49
1:A:156:GLY:O	1:A:179:PRO:HG2	2.12	0.49
1:B:142:GLU:HG2	1:B:144:LEU:CD2	2.44	0.48
1:C:128:ASN:O	1:C:130:ASP:N	2.47	0.48
1:A:122:VAL:HB	1:A:193:LEU:HD12	1.95	0.47
1:B:98:ASP:O	1:B:100:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:GLN:OE1	1:B:108:LEU:HA	2.15	0.47
1:C:127:ASP:O	1:C:186:LYS:HA	2.14	0.46
1:A:137:GLY:HA3	1:A:177:HIS:O	2.14	0.46
1:B:158:LYS:HE2	1:B:179:PRO:CB	2.45	0.46
1:A:16:LYS:HB2	1:A:44:GLU:HG2	1.98	0.46
1:A:19:ARG:HG2	1:A:24:MET:O	2.16	0.46
1:B:97:ARG:NH2	4:B:1006:HOH:O	2.48	0.46
1:B:104:VAL:HB	1:B:123:ASP:HB2	1.97	0.46
1:A:84:ILE:CG2	1:A:85:GLN:N	2.79	0.45
1:B:141:ASN:HD22	1:B:176:GLU:H	1.62	0.45
1:C:97:ARG:HB2	1:C:102:TYR:CB	2.47	0.45
1:B:28:ALA:O	1:B:32:LEU:HB2	2.18	0.44
1:A:104:VAL:HG23	1:A:125:LEU:HD11	1.99	0.44
1:A:84:ILE:HG22	1:A:85:GLN:N	2.31	0.44
1:C:86:MET:O	1:C:89:GLU:HG2	2.17	0.44
1:B:117:LEU:HG	1:B:119:PRO:HD3	1.98	0.44
1:C:104:VAL:HG23	1:C:125:LEU:HD11	2.00	0.44
1:B:151:ILE:HD13	1:B:193:LEU:HD23	1.99	0.44
1:C:176:GLU:O	1:C:177:HIS:HB2	2.18	0.43
1:C:130:ASP:N	1:C:130:ASP:OD2	2.51	0.43
1:B:18:ARG:HB2	4:B:1026:HOH:O	2.17	0.43
1:C:129:PRO:O	1:C:154:LYS:NZ	2.50	0.43
1:A:93:LEU:C	1:A:93:LEU:HD13	2.44	0.43
1:B:158:LYS:H	1:B:158:LYS:CD	2.18	0.43
1:B:143:PHE:C	1:B:144:LEU:HD22	2.44	0.42
1:B:128:ASN:C	1:B:128:ASN:ND2	2.78	0.42
1:A:33:LEU:HD23	1:A:62:VAL:HG21	2.02	0.42
1:C:151:ILE:CD1	1:C:191:ALA:HB1	2.50	0.42
1:C:36:THR:OG1	1:C:38:GLU:HG2	2.21	0.41
1:B:142:GLU:HB3	1:B:174:VAL:HG13	2.01	0.41
1:A:97:ARG:O	1:A:100:VAL:HG13	2.19	0.41
1:B:158:LYS:HE2	1:B:179:PRO:HB2	2.03	0.41
1:C:118:VAL:HB	1:C:197:ASN:HB2	2.01	0.41
1:C:127:ASP:HB3	1:C:189:GLY:O	2.21	0.41
1:A:63:LEU:HD12	1:A:63:LEU:HA	1.94	0.40
1:B:124:VAL:HG13	4:B:1007:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1047:HOH:O	4:A:1052:HOH:O[2_765]	2.13	0.07

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	190/198 (96%)	178 (94%)	12 (6%)	0	100	100
1	B	191/198 (96%)	187 (98%)	4 (2%)	0	100	100
1	C	188/198 (95%)	181 (96%)	6 (3%)	1 (0%)	24	31
All	All	569/594 (96%)	546 (96%)	22 (4%)	1 (0%)	43	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	129	PRO

5.3.2 Protein sidechains [i](#)

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	152/160 (95%)	143 (94%)	9 (6%)	18	26
1	B	151/160 (94%)	141 (93%)	10 (7%)	15	21
1	C	152/160 (95%)	143 (94%)	9 (6%)	18	26
All	All	455/480 (95%)	427 (94%)	28 (6%)	16	24

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LEU
1	A	70	LEU
1	A	96	VAL
1	A	100	VAL
1	A	148	GLU
1	A	158	LYS
1	A	159	GLU
1	A	160	ASN
1	A	172	MET
1	B	32	LEU
1	B	82	VAL
1	B	97	ARG
1	B	101	ASP
1	B	126	THR
1	B	144	LEU
1	B	148	GLU
1	B	158	LYS
1	B	159	GLU
1	B	174	VAL
1	C	82	VAL
1	C	83	ILE
1	C	97	ARG
1	C	129	PRO
1	C	130	ASP
1	C	147	LEU
1	C	151	ILE
1	C	172	MET
1	C	186	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	197	ASN
1	B	21	GLN
1	B	45	ASN
1	B	128	ASN
1	B	141	ASN
1	C	106	ASN
1	C	160	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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$
3	S0H	C	1002	2	7,7,7	4.55	4 (57%)	6,10,10	2.46	1 (16%)
3	S0H	B	1003	2	7,7,7	4.37	4 (57%)	6,10,10	2.47	1 (16%)
3	S0H	A	1001	2	7,7,7	4.35	4 (57%)	6,10,10	2.42	2 (33%)

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	S0H	C	1002	2	-	0/5/5/5	-
3	S0H	B	1003	2	-	0/5/5/5	-
3	S0H	A	1001	2	-	1/5/5/5	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1002	S0H	C1-C3	-9.85	1.10	1.51
3	A	1001	S0H	C1-C3	-9.64	1.11	1.51
3	B	1003	S0H	C1-C3	-9.61	1.11	1.51
3	C	1002	S0H	P1-C2	4.70	1.83	1.79
3	A	1001	S0H	P1-O13	-4.46	1.45	1.55
3	B	1003	S0H	P1-O13	-4.31	1.45	1.55
3	C	1002	S0H	P1-O13	-4.28	1.45	1.55
3	B	1003	S0H	P1-C2	3.80	1.83	1.79
3	A	1001	S0H	P1-C2	3.31	1.82	1.79
3	A	1001	S0H	P1-O14	2.85	1.56	1.50
3	B	1003	S0H	P1-O14	2.79	1.55	1.50
3	C	1002	S0H	P1-O14	2.60	1.55	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1003	S0H	O15-P1-O14	-5.33	98.59	112.39
3	C	1002	S0H	O15-P1-O14	-5.31	98.65	112.39
3	A	1001	S0H	O15-P1-O14	-4.99	99.49	112.39
3	A	1001	S0H	O15-P1-O13	2.15	114.08	107.96

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	S0H	P1-C2-C3-O6

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	192/198 (96%)	0.53	9 (4%) 36 38	26, 36, 52, 63	0
1	B	193/198 (97%)	0.62	14 (7%) 21 23	22, 37, 53, 57	0
1	C	192/198 (96%)	0.22	6 (3%) 51 53	17, 31, 47, 58	0
All	All	577/594 (97%)	0.45	29 (5%) 34 35	17, 35, 52, 63	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	148	GLU	5.3
1	C	98	ASP	5.2
1	A	160	ASN	3.9
1	B	6	THR	3.7
1	A	157	ASP	3.0
1	B	32	LEU	3.0
1	C	165	LEU	3.0
1	B	38	GLU	2.9
1	B	99	ASN	2.9
1	B	50	GLU	2.7
1	A	123	ASP	2.7
1	C	79	ASP	2.7
1	A	98	ASP	2.6
1	B	80	ASP	2.6
1	A	148	GLU	2.5
1	A	7	ALA	2.5
1	B	37	PRO	2.5
1	A	80	ASP	2.5
1	A	159	GLU	2.5
1	C	160	ASN	2.4
1	B	58	ARG	2.4
1	B	26	HIS	2.3
1	B	25	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	194	ILE	2.1
1	B	150	GLU	2.1
1	C	80	ASP	2.0
1	C	130	ASP	2.0
1	B	47	GLU	2.0
1	A	99	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($\text{\AA}^2$)	Q<0.9
3	S0H	B	1003	8/8	0.96	0.08	25,31,32,32	0
3	S0H	A	1001	8/8	0.97	0.08	32,33,35,38	0
3	S0H	C	1002	8/8	0.98	0.07	29,33,34,35	0
2	FE2	A	199	1/1	0.99	0.04	31,31,31,31	0
2	FE2	C	199	1/1	1.00	0.03	29,29,29,29	0
2	FE2	B	199	1/1	1.00	0.03	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.