



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:00 PM UTC

PDB ID : 5F4Z / pdb_00005f4z
Title : The crystal structure of an epoxide hydrolase from *Streptomyces carzinostaticus* subsp. *neocarzinostaticus*
Authors : Tan, K.; Li, H.; Jedrzejczak, R.; BABNIGG, G.; BINGMAN, C.A.; YEN-NAMALLI, R.; LOHMAN, J.; Chang, C.Y.; Shen, B.; Phillips Jr., G.N.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG); Enzyme Discovery for Natural Product Biosynthesis (NatPro)
Deposited on : 2015-12-03
Resolution : 1.82 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:

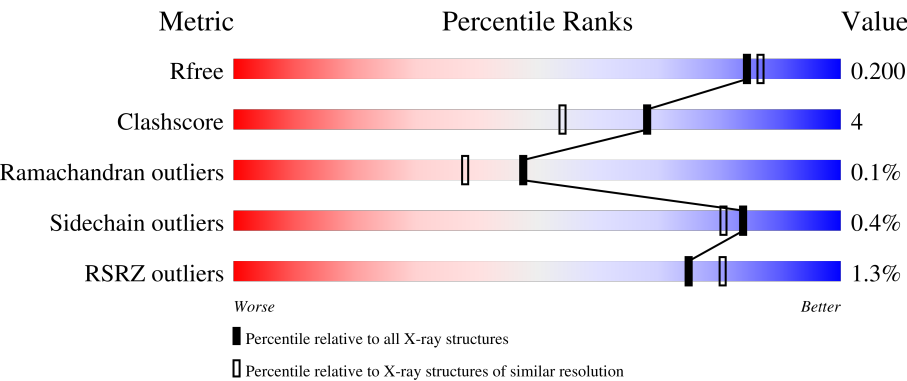
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	393	2% 92% 6% ..
1	B	393	% 91% 8% .
1	C	393	% 91% 8% .
1	D	393	2% 87% 12% ..

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Mol	Chain	Length	Quality of chain
1	E	393	%  94% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	A	406	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16650 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 Epoxide hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	Se	0	4	0
			3052	1958	525	562	7			
1	B	390	Total	C	N	O	Se	0	1	0
			3051	1956	526	562	7			
1	C	387	Total	C	N	O	Se	0	5	0
			3047	1953	525	562	7			
1	D	391	Total	C	N	O	Se	0	4	0
			3078	1972	533	566	7			
1	E	388	Total	C	N	O	Se	0	3	0
			3040	1949	522	562	7			

There are 30 discrepancies between the modelled and reference sequences:

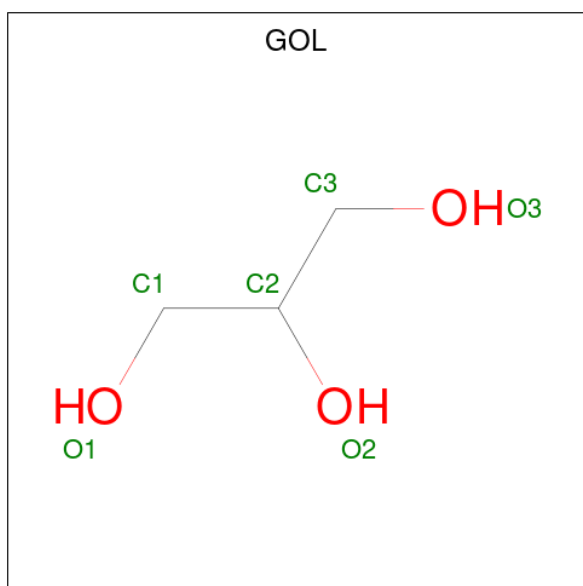
Chain	Residue	Modelled	Actual	Comment	Reference
A	388	HIS	-	expression tag	UNP Q84HB1
A	389	HIS	-	expression tag	UNP Q84HB1
A	390	HIS	-	expression tag	UNP Q84HB1
A	391	HIS	-	expression tag	UNP Q84HB1
A	392	HIS	-	expression tag	UNP Q84HB1
A	393	HIS	-	expression tag	UNP Q84HB1
B	388	HIS	-	expression tag	UNP Q84HB1
B	389	HIS	-	expression tag	UNP Q84HB1
B	390	HIS	-	expression tag	UNP Q84HB1
B	391	HIS	-	expression tag	UNP Q84HB1
B	392	HIS	-	expression tag	UNP Q84HB1
B	393	HIS	-	expression tag	UNP Q84HB1
C	388	HIS	-	expression tag	UNP Q84HB1
C	389	HIS	-	expression tag	UNP Q84HB1
C	390	HIS	-	expression tag	UNP Q84HB1
C	391	HIS	-	expression tag	UNP Q84HB1
C	392	HIS	-	expression tag	UNP Q84HB1
C	393	HIS	-	expression tag	UNP Q84HB1
D	388	HIS	-	expression tag	UNP Q84HB1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	389	HIS	-	expression tag	UNP Q84HB1
D	390	HIS	-	expression tag	UNP Q84HB1
D	391	HIS	-	expression tag	UNP Q84HB1
D	392	HIS	-	expression tag	UNP Q84HB1
D	393	HIS	-	expression tag	UNP Q84HB1
E	388	HIS	-	expression tag	UNP Q84HB1
E	389	HIS	-	expression tag	UNP Q84HB1
E	390	HIS	-	expression tag	UNP Q84HB1
E	391	HIS	-	expression tag	UNP Q84HB1
E	392	HIS	-	expression tag	UNP Q84HB1
E	393	HIS	-	expression tag	UNP Q84HB1

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



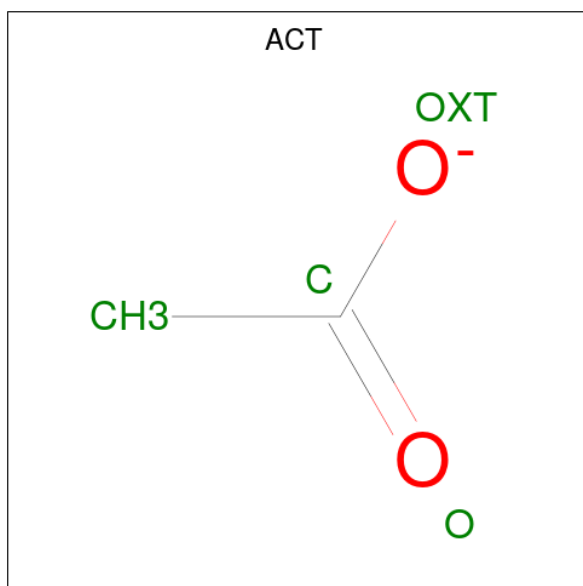
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		

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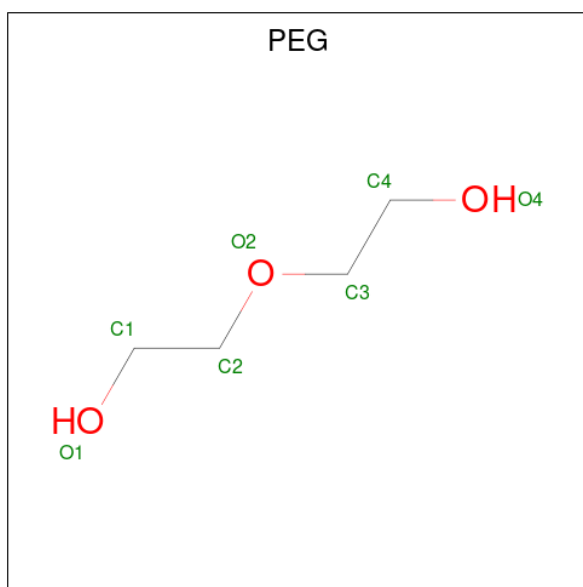
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



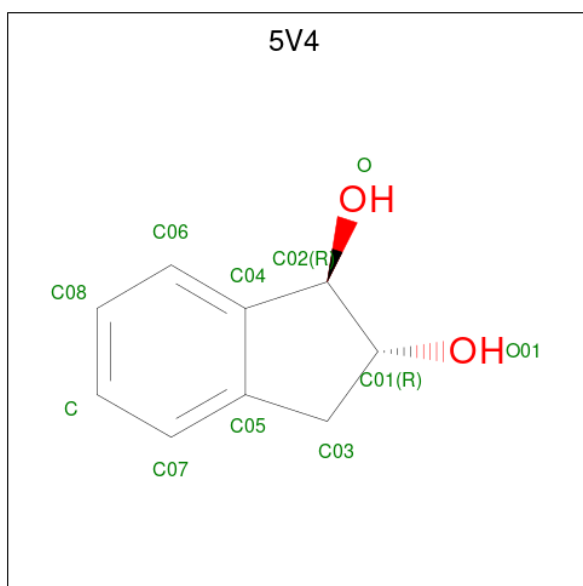
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $\text{C}_4\text{H}_{10}\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is (1 {R},2 {R})-2,3-dihydro-1 {H}-indene-1,2-diol (CCD ID: 5V4) (formula: C₉H₁₀O₂).



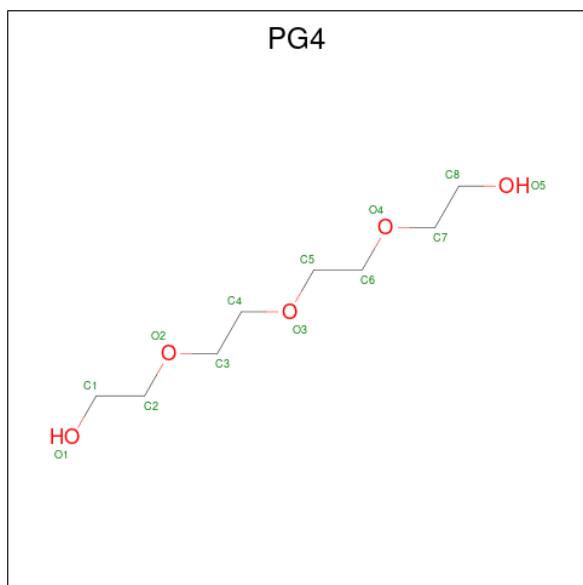
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	1
			22	18	4		
5	B	1	Total	C	O	0	1
			22	18	4		

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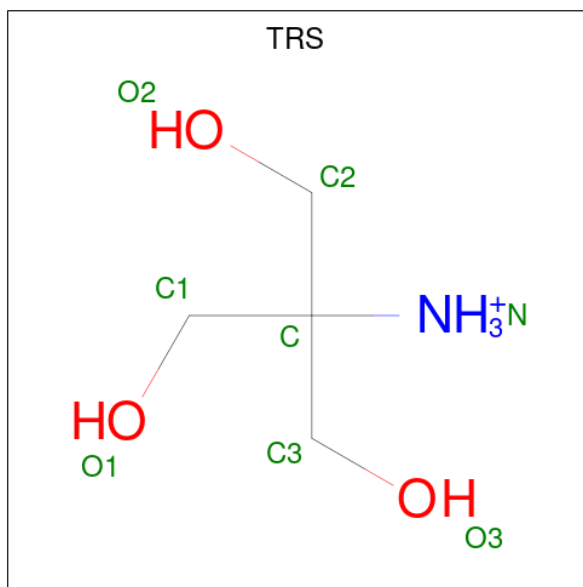
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	1
			22	18	4		
5	D	1	Total	C	O	0	1
			22	18	4		
5	E	1	Total	C	O	0	1
			22	18	4		

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			8	4	1	3		

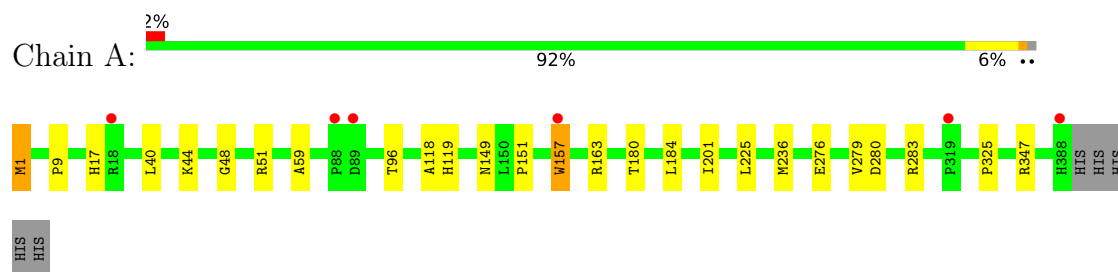
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	287	Total	O	0	1
			288	288		
8	B	256	Total	O	0	0
			256	256		
8	C	239	Total	O	0	1
			240	240		
8	D	191	Total	O	0	0
			191	191		
8	E	219	Total	O	0	0
			219	219		

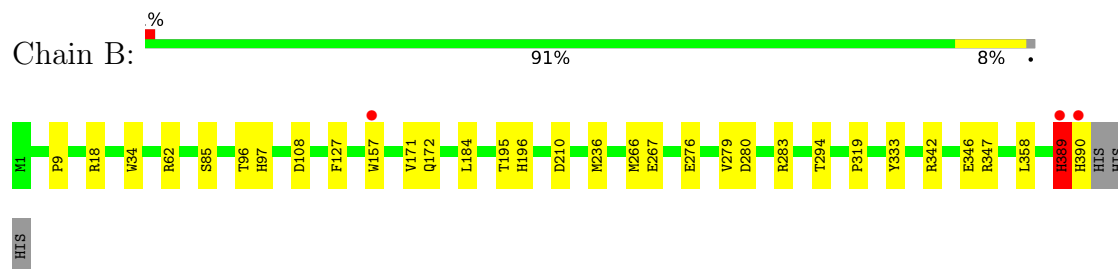
3 Residue-property plots [i](#)

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.

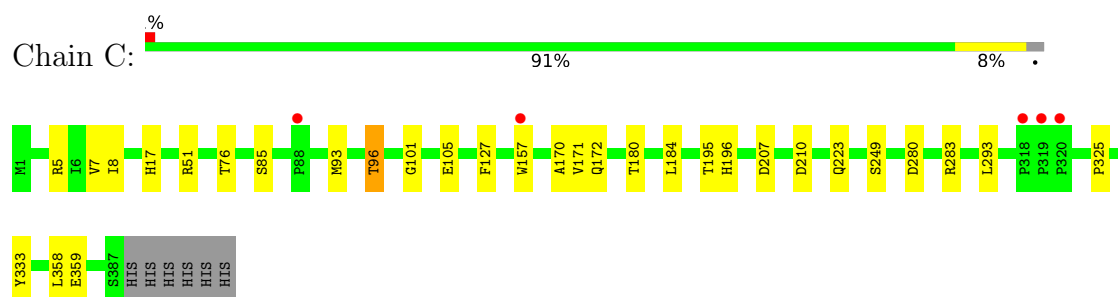
• Molecule 1: Epoxide hydrolase



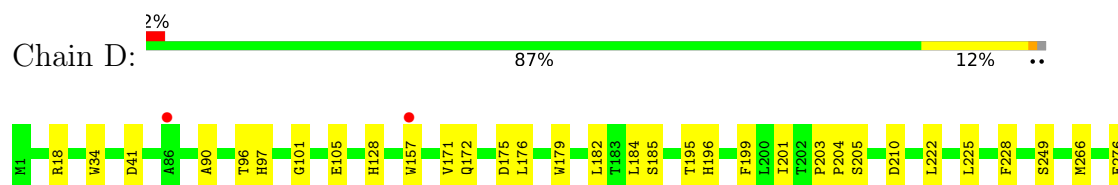
• Molecule 1: Epoxide hydrolase

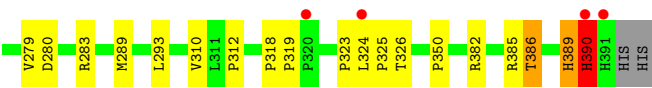


• Molecule 1: Epoxide hydrolase



• Molecule 1: Epoxide hydrolase





● Molecule 1: Epoxide hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	179.36Å 93.07Å 134.06Å 90.00° 115.33° 90.00°	Depositor
Resolution (Å)	33.27 – 1.82 33.27 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.27-1.82) 99.7 (33.27-1.82)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.82Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.160 , 0.200 0.162 , 0.200	Depositor DCC
R_{free} test set	8910 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16650	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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: GOL, ACT, PEG, PG4, 5V4, TRS

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	0.55	0/3158	0.78	1/4320 (0.0%)
1	B	0.51	0/3153	0.78	2/4315 (0.0%)
1	C	0.50	0/3155	0.77	1/4316 (0.0%)
1	D	0.46	0/3189	0.79	1/4362 (0.0%)
1	E	0.47	0/3145	0.75	1/4303 (0.0%)
All	All	0.50	0/15800	0.78	6/21616 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	TRP	N-CA-C	5.31	117.06	111.28
1	D	319	PRO	O-C-N	5.26	123.62	121.15
1	B	389	HIS	N-CA-C	5.22	118.81	112.23
1	B	319	PRO	O-C-N	5.11	123.66	121.31
1	E	96	THR	N-CA-C	5.10	117.21	108.90
1	C	96	THR	N-CA-C	5.07	116.67	108.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3052	0	2940	23	0
1	B	3051	0	2922	21	0
1	C	3047	0	2935	19	0
1	D	3078	0	2957	34	0
1	E	3040	0	2925	14	0
2	A	30	0	40	1	0
2	C	6	0	8	0	0
2	E	6	0	8	0	0
3	A	4	0	3	2	0
3	B	4	0	3	1	0
4	A	7	0	10	1	0
5	A	22	0	20	1	0
5	B	22	0	20	1	0
5	C	22	0	20	0	0
5	D	22	0	20	4	0
5	E	22	0	20	0	0
6	B	13	0	18	2	0
7	B	8	0	12	1	0
8	A	288	0	0	2	0
8	B	256	0	0	2	0
8	C	240	0	0	0	0
8	D	191	0	0	2	0
8	E	219	0	0	0	0
All	All	16650	0	14881	110	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 4.

All (110) 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:D:179[A]:TRP:CH2	5:D:401[A]:5V4:H9	2.14	0.82
1:B:157:TRP:HE3	1:B:184:LEU:HD22	1.48	0.77
1:A:157:TRP:HE3	1:A:184:LEU:HD22	1.50	0.75
1:A:325:PRO:HB3	1:C:325:PRO:HB3	1.78	0.66
1:A:59:ALA:HA	2:A:404:GOL:H32	1.78	0.65
1:D:324:LEU:HD12	1:D:325:PRO:HD2	1.79	0.64
1:A:96:THR:OG1	1:A:157:TRP:CH2	2.42	0.64
1:A:283:ARG:HH11	1:A:283:ARG:HG3	1.64	0.63
1:C:96:THR:OG1	1:C:157:TRP:CH2	2.41	0.62
1:D:157:TRP:HE3	1:D:184:LEU:HD22	1.64	0.62
1:E:96:THR:OG1	1:E:157:TRP:CH2	2.45	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MSE:HE1	1:A:163:ARG:HB3	1.82	0.61
1:B:342:ARG:O	1:B:346:GLU:HG2	2.02	0.60
1:A:347:ARG:NH2	8:A:503:HOH:O	2.36	0.58
1:C:280:ASP:OD2	1:C:283:ARG:NH1	2.37	0.56
1:E:96:THR:HG21	1:E:157:TRP:HH2	1.71	0.56
1:B:96:THR:OG1	1:B:157:TRP:CH2	2.45	0.56
1:B:389:HIS:CD2	1:B:389:HIS:C	2.84	0.54
1:C:96:THR:HG21	1:C:157:TRP:HH2	1.72	0.54
1:C:157:TRP:HE3	1:C:184:LEU:HD22	1.72	0.53
1:D:90:ALA:HB3	1:D:128:HIS:CD2	2.44	0.53
1:D:179[A]:TRP:CZ2	5:D:401[A]:5V4:H9	2.43	0.52
1:B:280:ASP:OD2	1:B:283:ARG:NH1	2.40	0.52
1:D:312:PRO:HG2	5:D:401[A]:5V4:H10	1.91	0.51
1:D:205:SER:OG	1:D:210:ASP:OD2	2.25	0.51
1:A:44:LYS:NZ	8:A:502:HOH:O	2.34	0.51
1:D:185:SER:OG	1:D:195:THR:OG1	2.26	0.50
1:A:40:LEU:HD11	1:A:44:LYS:HE3	1.94	0.50
1:A:280:ASP:OD2	1:A:283:ARG:NH1	2.44	0.50
1:B:18:ARG:HD2	8:B:541:HOH:O	2.11	0.50
1:C:96:THR:HG21	1:C:157:TRP:CH2	2.47	0.50
1:D:324:LEU:HG	1:D:326:THR:HG22	1.94	0.49
1:D:386:THR:O	1:D:389:HIS:HB3	2.12	0.49
1:B:276:GLU:HA	1:B:279:VAL:O	2.12	0.49
1:E:157:TRP:HE3	1:E:184:LEU:HD22	1.77	0.49
1:C:249:SER:HB2	1:D:249[B]:SER:HB3	1.95	0.48
1:B:9:PRO:HG2	6:B:402:PG4:H11	1.96	0.48
1:B:62:ARG:NH2	1:B:108:ASP:OD1	2.32	0.48
1:D:182:LEU:O	1:D:185:SER:HB2	2.14	0.47
1:A:48:GLY:HA2	3:A:406:ACT:H3	1.96	0.47
1:A:283:ARG:HG3	1:A:283:ARG:NH1	2.29	0.47
1:D:204:PRO:HD3	1:D:222:LEU:HD22	1.96	0.47
1:E:289:MSE:HE3	1:E:293:LEU:HD11	1.97	0.47
1:D:96:THR:HG22	1:D:97:HIS:O	2.15	0.47
1:C:333:TYR:CZ	1:C:358:LEU:HD13	2.50	0.46
1:E:96:THR:HG22	1:E:97:HIS:O	2.16	0.46
1:C:8:ILE:HG13	1:C:293:LEU:HD13	1.97	0.46
1:A:17:HIS:HB3	1:A:51:ARG:CZ	2.46	0.46
1:A:201[A]:ILE:HG23	1:A:225:LEU:HD11	1.97	0.46
1:C:157:TRP:CH2	1:C:180:THR:HG21	2.51	0.46
1:D:199:PHE:CZ	1:D:201:ILE:HD11	2.50	0.46
1:D:201:ILE:HG22	1:D:203:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ARG:HG2	3:A:406:ACT:OXT	2.16	0.45
1:A:96:THR:HG21	1:A:157:TRP:CH2	2.51	0.45
1:D:228:PHE:CE1	5:D:401[A]:5V4:H5	2.51	0.45
1:C:5[A]:ARG:HG2	1:C:7:VAL:HG23	1.99	0.45
1:D:101:GLY:HA3	1:D:105:GLU:OE2	2.17	0.45
1:A:9:PRO:HG2	4:A:407:PEG:H11	1.99	0.45
1:B:210:ASP:OD2	1:B:347:ARG:NH1	2.45	0.45
1:B:389:HIS:HD2	1:B:390:HIS:HD2	1.64	0.45
1:D:310:VAL:HA	1:D:318:PRO:HG3	1.99	0.45
1:E:96:THR:HG21	1:E:157:TRP:CH2	2.51	0.45
1:E:157:TRP:CH2	1:E:180:THR:HG21	2.53	0.44
1:D:41:ASP:HB2	8:D:670:HOH:O	2.17	0.44
1:D:382:ARG:HG2	1:D:385:ARG:NH1	2.32	0.44
1:B:333:TYR:CZ	1:B:358:LEU:HD13	2.52	0.44
1:C:101:GLY:HA3	1:C:105:GLU:OE2	2.18	0.44
1:A:118:ALA:O	1:A:119:HIS:HD2	2.01	0.44
3:B:401:ACT:H1	8:B:745:HOH:O	2.17	0.44
1:D:171:VAL:HG23	1:D:195:THR:HG23	2.00	0.43
1:D:289:MSE:HE3	1:D:293:LEU:HD11	1.99	0.43
1:E:101:GLY:HA3	1:E:105:GLU:OE2	2.18	0.43
1:E:112:PRO:HB2	1:E:374:VAL:HG21	2.01	0.43
1:B:389:HIS:HD2	1:B:390:HIS:CD2	2.36	0.43
1:E:90:ALA:HB3	1:E:128:HIS:NE2	2.33	0.43
1:B:294:THR:HA	6:B:402:PG4:H51	2.01	0.43
1:D:172:GLN:HA	1:D:196:HIS:O	2.19	0.43
1:D:386:THR:O	1:D:390:HIS:CD2	2.72	0.43
1:A:157:TRP:CH2	1:A:180:THR:HG21	2.54	0.43
1:A:96:THR:HG21	1:A:157:TRP:HH2	1.84	0.42
1:B:236:MSE:HE1	5:B:404[B]:5V4:H6	2.01	0.42
1:E:8:ILE:HG13	1:E:293:LEU:HD13	2.00	0.42
1:E:171:VAL:HG23	1:E:195:THR:HG23	2.02	0.42
1:B:34:TRP:CE3	1:B:266:MSE:HG2	2.53	0.42
1:D:18:ARG:HD2	8:D:624:HOH:O	2.18	0.42
1:B:85:SER:HB2	1:B:127:PHE:O	2.20	0.42
1:D:276:GLU:HA	1:D:279:VAL:O	2.20	0.42
1:A:149:ASN:CG	1:A:151:PRO:HD2	2.45	0.41
1:C:85:SER:HB2	1:C:127:PHE:O	2.21	0.41
1:C:93:MSE:HE3	1:C:170:ALA:HB1	2.02	0.41
1:D:175:ASP:CG	1:D:176:LEU:H	2.29	0.41
1:A:236:MSE:HE1	5:A:408[B]:5V4:H6	2.01	0.41
1:B:96:THR:HG22	1:B:97:HIS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:THR:CG2	1:C:157:TRP:CH2	3.03	0.41
1:D:323:PRO:HB3	1:D:350:PRO:HD3	2.03	0.41
1:D:390:HIS:CD2	1:D:390:HIS:H	2.38	0.41
1:C:17:HIS:HB3	1:C:51:ARG:CZ	2.51	0.41
1:C:172:GLN:HA	1:C:196:HIS:O	2.21	0.41
1:D:96:THR:HG21	1:D:157:TRP:CH2	2.56	0.41
1:D:225:LEU:HD23	1:D:225:LEU:HA	1.93	0.41
1:D:280:ASP:OD2	1:D:283:ARG:HD2	2.21	0.41
1:E:96:THR:CG2	1:E:157:TRP:HH2	2.34	0.41
1:A:276:GLU:HA	1:A:279:VAL:O	2.21	0.41
1:B:267:GLU:O	7:B:403:TRS:N	2.42	0.41
1:B:171:VAL:HG23	1:B:195:THR:HG23	2.03	0.40
1:B:172:GLN:HA	1:B:196:HIS:O	2.20	0.40
1:E:122:ASP:OD1	1:E:123:PRO:HD2	2.21	0.40
1:D:34:TRP:CE3	1:D:266:MSE:HG2	2.56	0.40
1:C:171:VAL:HG23	1:C:195:THR:HG23	2.04	0.40
1:C:207:ASP:O	1:C:210:ASP:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	390/393 (99%)	381 (98%)	9 (2%)	0	100	100
1	B	389/393 (99%)	375 (96%)	14 (4%)	0	100	100
1	C	390/393 (99%)	379 (97%)	11 (3%)	0	100	100
1	D	393/393 (100%)	378 (96%)	13 (3%)	2 (0%)	24	14
1	E	389/393 (99%)	379 (97%)	10 (3%)	0	100	100
All	All	1951/1965 (99%)	1892 (97%)	57 (3%)	2 (0%)	48	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	389	HIS
1	D	390	HIS

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	320/315 (102%)	319 (100%)	1 (0%)	86	84
1	B	319/315 (101%)	318 (100%)	1 (0%)	86	84
1	C	320/315 (102%)	317 (99%)	3 (1%)	70	62
1	D	323/315 (102%)	321 (99%)	2 (1%)	78	74
1	E	319/315 (101%)	319 (100%)	0	100	100
All	All	1601/1575 (102%)	1594 (100%)	7 (0%)	84	81

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	B	389	HIS
1	C	76	THR
1	C	223	GLN
1	C	359	GLU
1	D	386	THR
1	D	390	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	172	GLN
1	A	198	ASN
1	A	287	ASN

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Mol	Chain	Res	Type
1	B	119	HIS
1	B	172	GLN
1	B	198	ASN
1	B	389	HIS
1	B	390	HIS
1	C	68	GLN
1	C	172	GLN
1	C	198	ASN
1	D	351	ASN
1	D	390	HIS
1	E	217	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](#)

22 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	$\# Z > 2$
5	5V4	A	408[B]	-	12,12,12	4.32	8 (66%)	15,17,17	1.37	2 (13%)
7	TRS	B	403	-	7,7,7	0.33	0	9,9,9	0.64	0
3	ACT	B	401	-	3,3,3	0.79	0	3,3,3	1.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	5V4	A	408[A]	-	12,12,12	4.37	8 (66%)	15,17,17	1.75	3 (20%)
2	GOL	A	403	-	5,5,5	0.41	0	5,5,5	0.23	0
3	ACT	A	406	-	3,3,3	0.83	0	3,3,3	1.26	0
2	GOL	A	401	-	5,5,5	0.39	0	5,5,5	0.23	0
5	5V4	E	402[B]	-	12,12,12	4.31	8 (66%)	15,17,17	1.50	3 (20%)
5	5V4	B	404[B]	-	12,12,12	4.28	8 (66%)	15,17,17	1.48	2 (13%)
5	5V4	E	402[A]	-	12,12,12	4.35	8 (66%)	15,17,17	1.69	3 (20%)
5	5V4	B	404[A]	-	12,12,12	4.33	8 (66%)	15,17,17	1.59	3 (20%)
5	5V4	D	401[B]	-	12,12,12	4.38	8 (66%)	15,17,17	1.44	3 (20%)
4	PEG	A	407	-	6,6,6	0.63	0	5,5,5	0.67	0
6	PG4	B	402	-	12,12,12	0.94	0	11,11,11	0.25	0
5	5V4	D	401[A]	-	12,12,12	4.24	7 (58%)	15,17,17	1.53	4 (26%)
5	5V4	C	402[B]	-	12,12,12	4.40	8 (66%)	15,17,17	1.52	3 (20%)
5	5V4	C	402[A]	-	12,12,12	4.35	8 (66%)	15,17,17	1.64	3 (20%)
2	GOL	A	404	-	5,5,5	0.38	0	5,5,5	0.33	0
2	GOL	A	402	-	5,5,5	0.46	0	5,5,5	0.23	0
2	GOL	C	401	-	5,5,5	0.40	0	5,5,5	0.19	0
2	GOL	E	401	-	5,5,5	0.38	0	5,5,5	0.19	0
2	GOL	A	405	-	5,5,5	0.36	0	5,5,5	0.29	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
5	5V4	A	408[B]	-	-	-	0/2/2/2
7	TRS	B	403	-	-	8/9/9/9	-
5	5V4	A	408[A]	-	-	-	0/2/2/2
2	GOL	A	403	-	-	2/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-
5	5V4	E	402[B]	-	-	-	0/2/2/2
5	5V4	B	404[B]	-	-	-	0/2/2/2
5	5V4	E	402[A]	-	-	-	0/2/2/2
5	5V4	B	404[A]	-	-	-	0/2/2/2
5	5V4	D	401[B]	-	-	-	0/2/2/2
4	PEG	A	407	-	-	1/4/4/4	-
6	PG4	B	402	-	-	2/10/10/10	-
5	5V4	D	401[A]	-	-	-	0/2/2/2
5	5V4	C	402[B]	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	5V4	C	402[A]	-	-	-	0/2/2/2
2	GOL	A	404	-	-	2/4/4/4	-
2	GOL	A	402	-	-	2/4/4/4	-
2	GOL	C	401	-	-	2/4/4/4	-
2	GOL	E	401	-	-	4/4/4/4	-
2	GOL	A	405	-	-	4/4/4/4	-

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	402[B]	5V4	C01-C02	-8.37	1.44	1.53
5	C	402[A]	5V4	C01-C02	-8.27	1.44	1.53
5	D	401[A]	5V4	C01-C02	-8.25	1.44	1.53
5	D	401[B]	5V4	C01-C02	-8.16	1.44	1.53
5	E	402[B]	5V4	C01-C02	-8.16	1.44	1.53
5	E	402[A]	5V4	C01-C02	-8.13	1.45	1.53
5	B	404[A]	5V4	C01-C02	-8.05	1.45	1.53
5	A	408[A]	5V4	C01-C02	-8.01	1.45	1.53
5	A	408[B]	5V4	C01-C02	-7.98	1.45	1.53
5	B	404[B]	5V4	C01-C02	-7.97	1.45	1.53
5	A	408[A]	5V4	C06-C04	7.29	1.48	1.39
5	E	402[A]	5V4	C06-C04	7.16	1.48	1.39
5	C	402[B]	5V4	C06-C04	7.15	1.48	1.39
5	D	401[B]	5V4	C06-C04	7.14	1.48	1.39
5	B	404[B]	5V4	C06-C04	7.10	1.48	1.39
5	A	408[B]	5V4	C06-C04	7.09	1.48	1.39
5	B	404[A]	5V4	C06-C04	7.08	1.48	1.39
5	E	402[B]	5V4	C06-C04	7.01	1.48	1.39
5	C	402[A]	5V4	C06-C04	7.00	1.48	1.39
5	A	408[B]	5V4	C-C08	6.37	1.52	1.38
5	D	401[B]	5V4	C-C08	6.35	1.52	1.38
5	C	402[B]	5V4	C-C08	6.32	1.52	1.38
5	A	408[A]	5V4	C-C08	6.28	1.52	1.38
5	D	401[A]	5V4	C06-C04	6.25	1.47	1.39
5	B	404[A]	5V4	C-C08	6.23	1.51	1.38
5	E	402[A]	5V4	C-C08	6.23	1.51	1.38
5	E	402[B]	5V4	C-C08	6.17	1.51	1.38
5	B	404[B]	5V4	C-C08	6.16	1.51	1.38
5	D	401[A]	5V4	C-C08	6.03	1.51	1.38
5	C	402[A]	5V4	C-C08	5.99	1.51	1.38
5	D	401[B]	5V4	C07-C05	5.40	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	408[B]	5V4	C07-C05	5.39	1.48	1.39
5	B	404[A]	5V4	C07-C05	5.32	1.48	1.39
5	C	402[B]	5V4	C07-C05	5.29	1.48	1.39
5	C	402[A]	5V4	C07-C05	5.27	1.48	1.39
5	A	408[A]	5V4	C07-C05	5.24	1.48	1.39
5	B	404[B]	5V4	C07-C05	5.24	1.48	1.39
5	E	402[B]	5V4	C07-C05	5.19	1.48	1.39
5	E	402[A]	5V4	C07-C05	5.13	1.47	1.39
5	D	401[A]	5V4	C07-C05	5.11	1.47	1.39
5	C	402[A]	5V4	C03-C05	4.83	1.59	1.50
5	E	402[A]	5V4	C03-C05	4.67	1.59	1.50
5	A	408[A]	5V4	C03-C05	4.63	1.59	1.50
5	B	404[A]	5V4	C03-C05	4.60	1.59	1.50
5	C	402[B]	5V4	C03-C05	4.50	1.58	1.50
5	D	401[B]	5V4	C03-C05	4.49	1.58	1.50
5	B	404[B]	5V4	C03-C05	4.44	1.58	1.50
5	A	408[B]	5V4	C03-C05	4.42	1.58	1.50
5	E	402[B]	5V4	C03-C05	4.40	1.58	1.50
5	D	401[A]	5V4	C03-C05	4.17	1.58	1.50
5	D	401[A]	5V4	C04-C02	-3.51	1.46	1.51
5	D	401[B]	5V4	C03-C01	-2.82	1.49	1.53
5	E	402[B]	5V4	C03-C01	-2.80	1.49	1.53
5	A	408[A]	5V4	C04-C02	-2.80	1.47	1.51
5	C	402[A]	5V4	C04-C02	-2.78	1.47	1.51
5	E	402[A]	5V4	C04-C02	-2.77	1.47	1.51
5	A	408[B]	5V4	C03-C01	-2.74	1.49	1.53
5	B	404[A]	5V4	C04-C02	-2.69	1.47	1.51
5	C	402[B]	5V4	C03-C01	-2.68	1.49	1.53
5	D	401[A]	5V4	C03-C01	-2.68	1.49	1.53
5	E	402[A]	5V4	C03-C01	-2.64	1.49	1.53
5	B	404[B]	5V4	C03-C01	-2.63	1.49	1.53
5	A	408[A]	5V4	C03-C01	-2.61	1.49	1.53
5	C	402[A]	5V4	C03-C01	-2.54	1.49	1.53
5	E	402[B]	5V4	C04-C02	-2.50	1.47	1.51
5	C	402[B]	5V4	C04-C02	-2.45	1.47	1.51
5	B	404[A]	5V4	C03-C01	-2.43	1.50	1.53
5	D	401[B]	5V4	C04-C02	-2.41	1.48	1.51
5	B	404[B]	5V4	C04-C02	-2.37	1.48	1.51
5	A	408[B]	5V4	C04-C02	-2.33	1.48	1.51
5	D	401[B]	5V4	C-C07	2.25	1.42	1.38
5	A	408[A]	5V4	C-C07	2.20	1.42	1.38
5	C	402[B]	5V4	C-C07	2.19	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	402[A]	5V4	C-C07	2.15	1.42	1.38
5	E	402[B]	5V4	C-C07	2.14	1.42	1.38
5	B	404[B]	5V4	C-C07	2.13	1.42	1.38
5	B	404[A]	5V4	C-C07	2.12	1.42	1.38
5	E	402[A]	5V4	C-C07	2.08	1.42	1.38
5	A	408[B]	5V4	C-C07	2.04	1.42	1.38

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	408[A]	5V4	C05-C04-C02	-3.90	107.52	110.46
5	E	402[A]	5V4	C05-C04-C02	-3.89	107.53	110.46
5	B	404[B]	5V4	C05-C04-C02	-3.72	107.66	110.46
5	E	402[B]	5V4	C05-C04-C02	-3.71	107.66	110.46
5	D	401[B]	5V4	C05-C04-C02	-3.67	107.69	110.46
5	C	402[A]	5V4	C05-C04-C02	-3.67	107.69	110.46
5	A	408[A]	5V4	C05-C03-C01	-3.63	100.11	103.43
5	C	402[B]	5V4	C05-C04-C02	-3.59	107.75	110.46
5	A	408[B]	5V4	C05-C04-C02	-3.40	107.89	110.46
5	B	404[A]	5V4	C05-C04-C02	-3.34	107.94	110.46
5	B	404[A]	5V4	C05-C03-C01	-3.31	100.40	103.43
5	E	402[A]	5V4	C05-C03-C01	-3.26	100.45	103.43
5	C	402[A]	5V4	C05-C03-C01	-3.09	100.61	103.43
5	E	402[B]	5V4	C06-C04-C02	2.69	131.69	128.54
5	B	404[B]	5V4	C06-C04-C02	2.68	131.68	128.54
5	C	402[B]	5V4	C06-C04-C02	2.62	131.60	128.54
5	E	402[A]	5V4	C06-C04-C02	2.59	131.57	128.54
5	D	401[B]	5V4	C06-C04-C02	2.54	131.51	128.54
5	A	408[A]	5V4	C06-C04-C02	2.53	131.50	128.54
5	C	402[B]	5V4	C05-C03-C01	-2.48	101.16	103.43
5	B	404[A]	5V4	C06-C04-C02	2.41	131.36	128.54
5	E	402[B]	5V4	C05-C03-C01	-2.39	101.25	103.43
5	D	401[A]	5V4	C05-C04-C02	-2.33	108.70	110.46
5	D	401[A]	5V4	C05-C03-C01	-2.28	101.34	103.43
5	A	408[B]	5V4	C06-C04-C02	2.25	131.18	128.54
5	D	401[A]	5V4	C08-C06-C04	-2.13	118.44	120.99
5	C	402[A]	5V4	C06-C04-C02	2.12	131.03	128.54
5	D	401[A]	5V4	C-C08-C06	2.06	122.78	120.24
5	D	401[B]	5V4	C05-C03-C01	-2.01	101.60	103.43

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	GOL	O1-C1-C2-C3
2	A	403	GOL	O1-C1-C2-C3
2	A	405	GOL	O1-C1-C2-C3
2	C	401	GOL	O1-C1-C2-C3
2	E	401	GOL	O1-C1-C2-O2
2	E	401	GOL	O1-C1-C2-C3
7	B	403	TRS	N-C-C1-O1
7	B	403	TRS	N-C-C2-O2
6	B	402	PG4	C4-C3-O2-C2
2	A	403	GOL	O1-C1-C2-O2
2	A	405	GOL	C1-C2-C3-O3
2	E	401	GOL	C1-C2-C3-O3
2	A	405	GOL	O1-C1-C2-O2
2	C	401	GOL	O1-C1-C2-O2
6	B	402	PG4	O4-C7-C8-O5
7	B	403	TRS	N-C-C3-O3
2	A	402	GOL	O1-C1-C2-O2
2	A	404	GOL	O1-C1-C2-C3
7	B	403	TRS	C3-C-C2-O2
7	B	403	TRS	C1-C-C3-O3
7	B	403	TRS	C2-C-C3-O3
2	A	405	GOL	O2-C2-C3-O3
4	A	407	PEG	C4-C3-O2-C2
7	B	403	TRS	C2-C-C1-O1
2	A	404	GOL	O1-C1-C2-O2
2	E	401	GOL	O2-C2-C3-O3
7	B	403	TRS	C1-C-C2-O2

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	408[B]	5V4	1	0
7	B	403	TRS	1	0
3	B	401	ACT	1	0
3	A	406	ACT	2	0
5	B	404[B]	5V4	1	0
4	A	407	PEG	1	0
6	B	402	PG4	2	0
5	D	401[A]	5V4	4	0
2	A	404	GOL	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	381/393 (96%)	-0.48	6 (1%) 70 77	13, 23, 48, 98	4 (1%)
1	B	383/393 (97%)	-0.45	3 (0%) 82 87	14, 26, 54, 105	1 (0%)
1	C	380/393 (96%)	-0.37	5 (1%) 75 80	13, 27, 56, 83	5 (1%)
1	D	384/393 (97%)	-0.21	6 (1%) 70 77	15, 34, 65, 106	4 (1%)
1	E	381/393 (96%)	-0.30	5 (1%) 75 80	16, 30, 54, 84	3 (0%)
All	All	1909/1965 (97%)	-0.36	25 (1%) 75 80	13, 28, 58, 106	17 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	TRP	5.8
1	D	157	TRP	4.6
1	C	157	TRP	4.5
1	E	157	TRP	4.4
1	B	157	TRP	4.1
1	A	388	HIS	4.1
1	E	388	HIS	3.4
1	E	320	PRO	3.3
1	C	320	PRO	2.7
1	D	320	PRO	2.7
1	E	321	ALA	2.7
1	A	89	ASP	2.7
1	D	324	LEU	2.7
1	B	389	HIS	2.6
1	D	391	HIS	2.6
1	A	319	PRO	2.6
1	D	390	HIS	2.5
1	A	18[A]	ARG	2.5
1	C	318	PRO	2.4
1	D	86	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	88	PRO	2.2
1	E	210	ASP	2.2
1	A	88	PRO	2.2
1	B	390	HIS	2.1
1	C	319	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PEG	A	407	7/7	0.65	0.17	71,72,74,76	0
7	TRS	B	403	8/8	0.69	0.15	34,49,58,60	0
5	5V4	D	401[B]	11/11	0.72	0.12	32,36,40,41	11
5	5V4	D	401[A]	11/11	0.72	0.12	30,36,39,42	11
6	PG4	B	402	13/13	0.74	0.17	46,73,80,81	0
2	GOL	C	401	6/6	0.77	0.14	51,64,66,72	0
2	GOL	A	403	6/6	0.79	0.14	60,63,65,66	0
2	GOL	A	401	6/6	0.80	0.11	41,59,62,62	0
2	GOL	A	405	6/6	0.82	0.12	67,69,69,70	0
5	5V4	A	408[A]	11/11	0.85	0.10	21,25,28,30	11
5	5V4	A	408[B]	11/11	0.85	0.10	18,23,27,30	11
3	ACT	A	406	4/4	0.85	0.14	54,55,58,61	0
3	ACT	B	401	4/4	0.86	0.14	50,59,59,61	0
2	GOL	A	404	6/6	0.86	0.13	66,69,71,73	0
2	GOL	E	401	6/6	0.87	0.10	50,57,64,66	0
5	5V4	E	402[A]	11/11	0.90	0.09	28,30,33,33	11
5	5V4	E	402[B]	11/11	0.90	0.09	26,30,33,33	11
5	5V4	B	404[A]	11/11	0.91	0.09	24,29,31,31	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	5V4	B	404[B]	11/11	0.91	0.09	26,29,33,34	11
2	GOL	A	402	6/6	0.94	0.07	31,45,45,53	0
5	5V4	C	402[A]	11/11	0.96	0.06	23,28,30,31	11
5	5V4	C	402[B]	11/11	0.96	0.06	26,30,32,33	11

6.5 Other polymers [i](#)

There are no such residues in this entry.