



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:25 PM UTC

PDB ID : 9IIA / pdb_00009iia
Title : Crystal structure of the free histidine prenyltransferase FunA
Authors : Chen, X.; Liu, Z.; Dai, S.; Zou, Y.
Deposited on : 2024-06-19
Resolution : 2.27 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

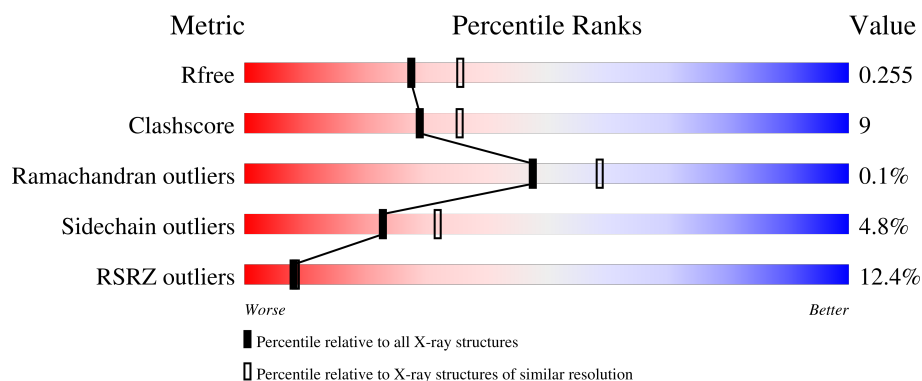
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	441	
1	B	441	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6758 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.

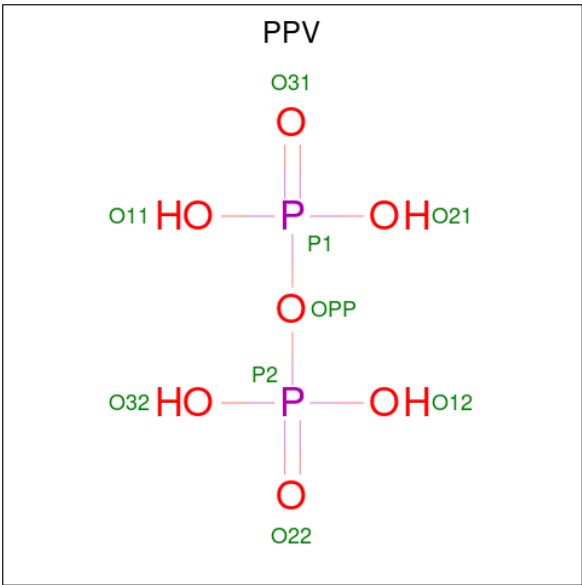
- Molecule 1 is a protein called Dimethylallyl tryptophan synthase GliD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	55	1	0
			3351	2140	567	625	19			
1	B	412	Total	C	N	O	S	134	1	0
			3257	2082	550	607	18			

There are 12 discrepancies between the modelled and reference sequences:

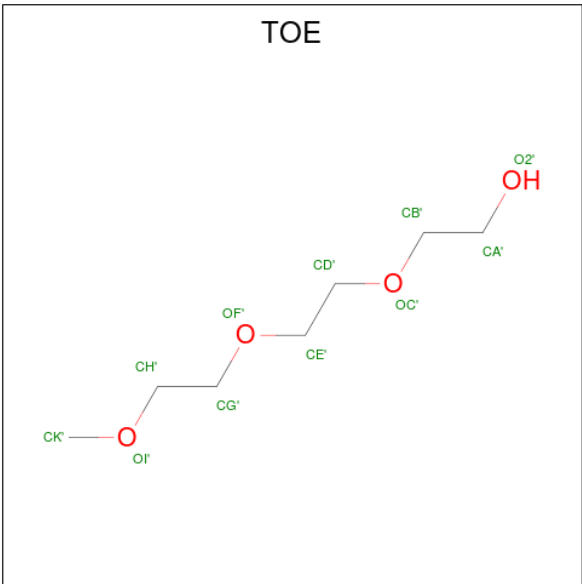
Chain	Residue	Modelled	Actual	Comment	Reference
A	5	SER	ASN	conflict	UNP A0A8K0WD55
A	82	GLU	LYS	conflict	UNP A0A8K0WD55
A	189	ASN	SER	conflict	UNP A0A8K0WD55
A	224	GLN	GLU	conflict	UNP A0A8K0WD55
A	230	ILE	MET	conflict	UNP A0A8K0WD55
A	335	PRO	SER	conflict	UNP A0A8K0WD55
B	5	SER	ASN	conflict	UNP A0A8K0WD55
B	82	GLU	LYS	conflict	UNP A0A8K0WD55
B	189	ASN	SER	conflict	UNP A0A8K0WD55
B	224	GLN	GLU	conflict	UNP A0A8K0WD55
B	230	ILE	MET	conflict	UNP A0A8K0WD55
B	335	PRO	SER	conflict	UNP A0A8K0WD55

- Molecule 2 is PYROPHOSPHATE (CCD ID: PPV) (formula: $\text{H}_4\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			9	7	2		
2	B	1	Total	O	P	0	0
			9	7	2		

- Molecule 3 is 2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXYL (CCD ID: TOE) (formula: C₇H₁₆O₄).



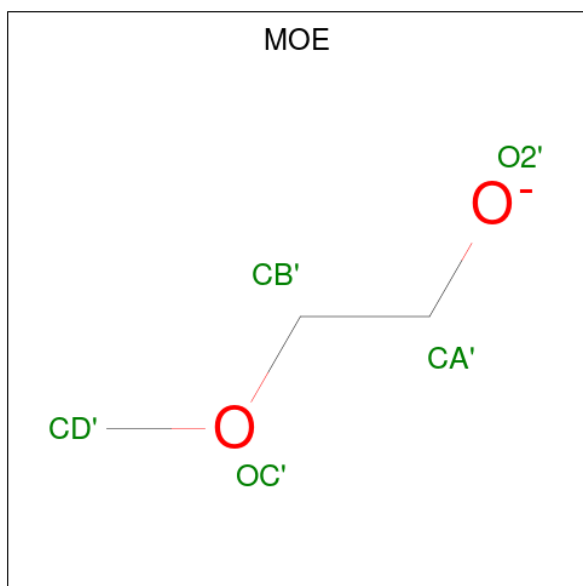
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	7	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			11	7	4		

- Molecule 4 is METHOXY-ETHOXYL (CCD ID: MOE) (formula: $C_3H_7O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			5	3	2		

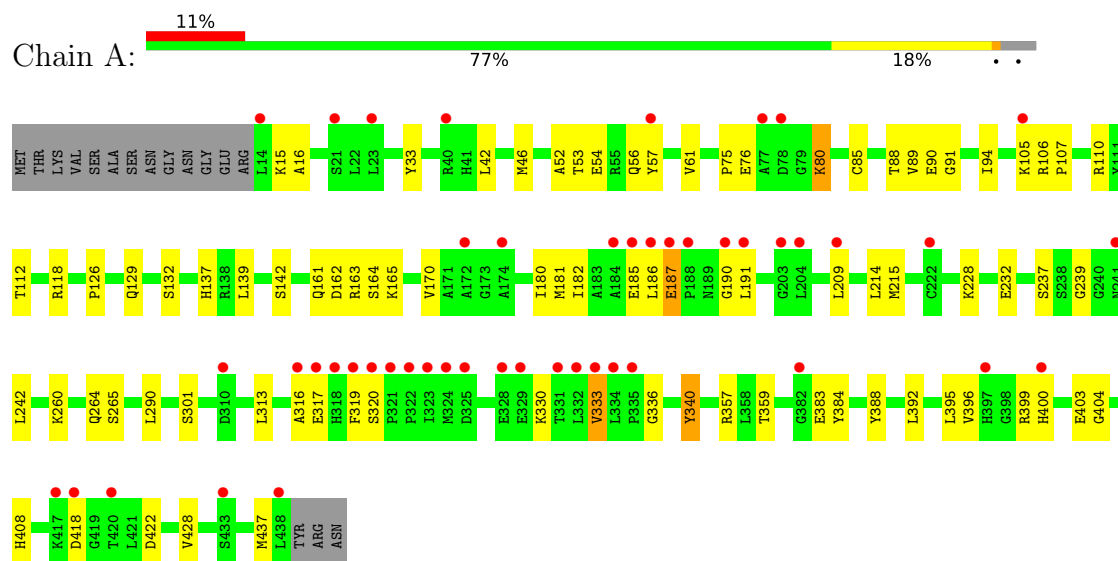
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	48	Total	O	0	0
			48	48		
5	B	57	Total	O	0	0
			57	57		

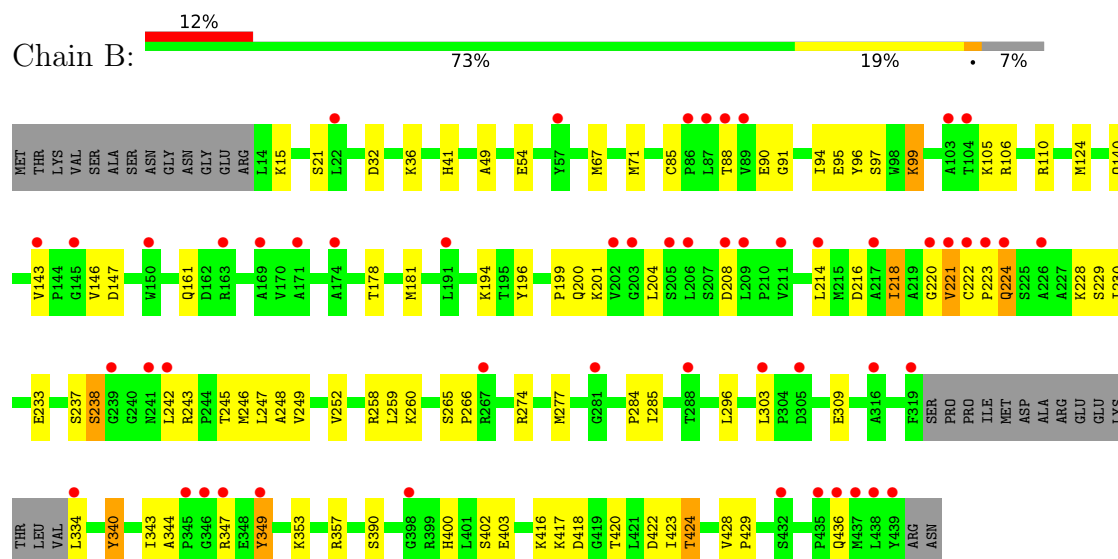
3 Residue-property plots [i](#)

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: Dimethylallyl tryptophan synthase GliD1



• Molecule 1: Dimethylallyl tryptophan synthase GliD1



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	202.21Å 202.21Å 111.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.45 – 2.27 31.45 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.8 (31.45-2.27) 99.8 (31.45-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.26Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.213 , 0.252 0.223 , 0.255	Depositor DCC
R_{free} test set	2000 reflections (3.23%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6758	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MOE, TOE, PPV

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	0.40	0/3443	0.60	2/4685 (0.0%)
1	B	0.41	0/3347	0.62	4/4553 (0.1%)
All	All	0.41	0/6790	0.61	6/9238 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	TYR	N-CA-C	6.79	121.64	112.88
1	B	303	LEU	N-CA-C	6.29	117.86	110.31
1	B	349	TYR	N-CA-C	5.65	115.40	108.11
1	A	316	ALA	N-CA-C	-5.46	102.80	110.50
1	B	178	THR	N-CA-C	5.30	118.16	110.42
1	B	218	ILE	N-CA-C	-5.02	104.66	111.89

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3351	0	3292	54	0
1	B	3257	0	3189	59	0
2	A	9	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	9	0	0	0	0
3	A	11	0	16	1	0
3	B	11	0	16	4	0
4	B	5	0	7	1	0
5	A	48	0	0	0	0
5	B	57	0	0	0	0
All	All	6758	0	6520	112	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 9.

All (112) 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:222:CYS:HB2	1:B:228:LYS:HE2	1.55	0.88
1:B:88:THR:HG22	1:B:90:GLU:H	1.38	0.85
1:A:162:ASP:HB3	1:A:165:LYS:HD2	1.62	0.80
1:A:88:THR:HG22	1:A:90:GLU:H	1.49	0.78
1:B:243:ARG:NH1	1:B:266:PRO:HD3	2.00	0.77
1:B:196:TYR:HB3	1:B:246:MET:CE	2.16	0.75
1:B:196:TYR:HB3	1:B:246:MET:HE1	1.68	0.74
1:B:222:CYS:O	1:B:228:LYS:HE3	1.89	0.72
1:A:319:PHE:HE1	1:A:404:GLY:HA2	1.56	0.70
1:B:105:LYS:HA	1:B:105:LYS:HE2	1.77	0.67
1:B:99:LYS:HA	1:B:424:THR:HB	1.79	0.64
1:A:186:LEU:HA	1:A:191:LEU:HD22	1.80	0.63
1:A:89:VAL:HG21	1:A:437:MET:HE2	1.81	0.63
1:B:181:MET:HE1	3:B:503:TOE:H14	1.81	0.62
1:B:237:SER:OG	1:B:238:SER:N	2.34	0.60
1:A:88:THR:HG22	1:A:90:GLU:N	2.17	0.60
1:A:190:GLY:O	1:A:191:LEU:HD23	2.01	0.60
1:B:417:LYS:HD3	1:B:417:LYS:H	1.67	0.59
1:B:247:LEU:HD12	1:B:248:ALA:N	2.18	0.58
1:B:54:GLU:CD	1:B:54:GLU:H	2.13	0.57
1:B:85:CYS:O	1:B:91:GLY:HA2	2.05	0.56
1:B:229:SER:O	1:B:233:GLU:HG3	2.05	0.56
1:A:264:GLN:OE1	1:A:357:ARG:NH1	2.27	0.56
1:B:242:LEU:HD23	1:B:265:SER:HB2	1.88	0.56
1:A:228:LYS:O	1:A:232:GLU:HG2	2.05	0.56
1:A:161:GLN:HG3	1:B:161:GLN:HG3	1.88	0.55
1:A:137:HIS:CG	1:B:124:MET:HB2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:HIS:HB2	1:B:403:GLU:HG3	1.89	0.54
1:B:220:GLY:O	1:B:222:CYS:N	2.37	0.54
1:A:396:VAL:HG21	1:A:399:ARG:HG2	1.90	0.53
1:A:400:HIS:HB2	1:A:403:GLU:OE2	2.09	0.53
1:A:209:LEU:HD13	1:A:214:LEU:HD21	1.90	0.52
1:B:96:TYR:CE2	1:B:429:PRO:HD3	2.45	0.52
1:B:99:LYS:HE3	1:B:422:ASP:OD2	2.10	0.52
1:A:105:LYS:HE3	1:A:106:ARG:H	1.76	0.51
1:B:181:MET:HE1	3:B:503:TOE:CK'	2.41	0.51
1:B:199:PRO:HG2	1:B:214:LEU:HG	1.93	0.51
1:A:85:CYS:O	1:A:91:GLY:HA2	2.11	0.50
1:B:230:ILE:HD12	1:B:230:ILE:H	1.75	0.50
1:B:194:LYS:HE3	1:B:196:TYR:OH	2.12	0.49
1:A:388:TYR:OH	1:A:408:HIS:NE2	2.36	0.48
1:B:343:ILE:O	1:B:343:ILE:HD12	2.13	0.48
1:B:347:ARG:HD3	1:B:349:TYR:O	2.13	0.48
1:B:245:THR:HB	4:B:502:MOE:HB'1	1.95	0.48
1:B:201:LYS:HB2	1:B:208:ASP:O	2.14	0.48
1:A:129:GLN:HG2	1:A:180:ILE:HD12	1.95	0.47
1:B:249:VAL:HG12	1:B:259:LEU:HD12	1.95	0.47
1:B:296:LEU:HD22	1:B:423:ILE:HD12	1.96	0.47
1:A:185:GLU:HB3	1:A:187:GLU:CG	2.44	0.47
1:A:186:LEU:HA	1:A:191:LEU:CD2	2.42	0.47
1:B:15:LYS:C	1:B:15:LYS:HD3	2.40	0.47
1:B:417:LYS:H	1:B:417:LYS:CD	2.27	0.47
1:A:242:LEU:CD2	1:A:265:SER:HB2	2.45	0.46
1:B:220:GLY:C	1:B:222:CYS:H	2.22	0.46
1:A:215:MET:HB2	1:A:215:MET:HE2	1.81	0.46
1:B:196:TYR:HB3	1:B:246:MET:HE2	1.97	0.46
1:A:317:GLU:O	1:A:319:PHE:N	2.43	0.46
1:B:334:LEU:O	1:B:357:ARG:NH1	2.43	0.46
1:A:237:SER:C	1:A:239:GLY:H	2.23	0.46
1:B:418:ASP:OD1	1:B:420:THR:HG23	2.16	0.45
1:A:181:MET:HE1	3:A:502:TOE:H15	1.98	0.45
1:A:242:LEU:HD23	1:A:265:SER:HB2	1.99	0.45
3:B:503:TOE:H12	3:B:503:TOE:H9	1.61	0.45
1:A:16:ALA:HA	1:A:57:TYR:CE1	2.51	0.45
1:A:319:PHE:O	1:A:320:SER:C	2.60	0.45
1:B:32:ASP:O	1:B:36:LYS:HG3	2.17	0.44
1:A:110:ARG:HE	1:A:110:ARG:HB2	1.59	0.44
1:B:41:HIS:CE1	1:B:429:PRO:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ARG:HA	1:B:344:ALA:HB2	1.99	0.44
1:A:42:LEU:O	1:A:46:MET:HG3	2.17	0.44
1:B:67:MET:O	1:B:71:MET:HG3	2.18	0.44
1:B:260:LYS:HD3	1:B:340:TYR:CE2	2.53	0.43
1:A:76:GLU:OE1	1:A:80:LYS:HG2	2.18	0.43
1:A:333:VAL:HG13	1:A:359:THR:HG22	2.01	0.43
1:A:106:ARG:HG3	1:A:107:PRO:O	2.19	0.43
1:A:185:GLU:HB3	1:A:187:GLU:HG2	2.00	0.43
1:A:330:LYS:HB3	1:A:330:LYS:HE2	1.88	0.43
1:B:353:LYS:HE3	1:B:353:LYS:HB2	1.76	0.43
1:B:274:ARG:HH21	1:B:309:GLU:CD	2.26	0.43
1:A:132:SER:HB3	1:A:182:ILE:HD11	1.99	0.43
1:A:340:TYR:C	1:A:340:TYR:CD1	2.96	0.43
1:A:139:LEU:HD23	1:A:139:LEU:HA	1.89	0.43
1:A:162:ASP:HB3	1:A:165:LYS:CD	2.41	0.43
1:B:340:TYR:C	1:B:340:TYR:CD1	2.97	0.43
1:A:110:ARG:HD2	1:A:185:GLU:HG2	1.99	0.43
1:A:418:ASP:OD1	1:A:418:ASP:N	2.35	0.43
1:B:334:LEU:O	1:B:357:ARG:NH2	2.50	0.42
1:B:416:LYS:HE3	1:B:416:LYS:HB3	1.73	0.42
1:B:49:ALA:O	1:B:106:ARG:HD3	2.20	0.42
1:B:97:SER:OG	1:B:110:ARG:NE	2.36	0.42
1:B:147:ASP:HB3	1:B:252:VAL:C	2.45	0.42
1:A:52:ALA:O	1:A:56:GLN:HG3	2.20	0.42
1:A:260:LYS:NZ	2:A:501:PPV:O32	2.52	0.42
1:B:223:PRO:O	1:B:224:GLN:C	2.63	0.42
1:A:15:LYS:HD3	1:A:53:THR:HG21	2.01	0.42
1:B:296:LEU:CD2	1:B:423:ILE:HD12	2.49	0.42
1:A:94:ILE:HA	1:A:112:THR:O	2.20	0.41
1:A:54:GLU:H	1:A:54:GLU:CD	2.27	0.41
1:B:284:PRO:O	1:B:285:ILE:HD13	2.20	0.41
1:A:126:PRO:HD2	1:A:163[A]:ARG:HD3	2.02	0.41
1:A:317:GLU:C	1:A:319:PHE:N	2.79	0.41
1:B:95:GLU:OE1	3:B:503:TOE:H8	2.20	0.41
1:A:110:ARG:HG2	1:A:185:GLU:HA	2.01	0.41
1:B:247:LEU:HD12	1:B:248:ALA:H	1.85	0.41
1:B:140:GLN:HA	1:B:146:VAL:HB	2.01	0.41
1:A:399:ARG:HG3	1:A:400:HIS:O	2.21	0.40
1:A:265:SER:O	1:A:336:GLY:HA3	2.21	0.40
1:A:290:LEU:HD23	1:A:290:LEU:HA	1.92	0.40
1:B:243:ARG:CZ	1:B:266:PRO:HD3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:TYR:CE2	1:A:75:PRO:HD2	2.57	0.40
1:B:344:ALA:HB3	1:B:347:ARG:NH1	2.36	0.40
1:A:162:ASP:CB	1:A:165:LYS:HD2	2.40	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	424/441 (96%)	404 (95%)	20 (5%)	0	100	100
1	B	409/441 (93%)	387 (95%)	21 (5%)	1 (0%)	43	53
All	All	833/882 (94%)	791 (95%)	41 (5%)	1 (0%)	48	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	221	VAL

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	362/375 (96%)	346 (96%)	16 (4%)	25	35
1	B	351/375 (94%)	333 (95%)	18 (5%)	21	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	713/750 (95%)	679 (95%)	34 (5%)	23	32

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	VAL
1	A	80	LYS
1	A	118	ARG
1	A	142	SER
1	A	164	SER
1	A	170	VAL
1	A	187	GLU
1	A	301	SER
1	A	313	LEU
1	A	333	VAL
1	A	340	TYR
1	A	383	GLU
1	A	392	LEU
1	A	395	LEU
1	A	422	ASP
1	A	428	VAL
1	B	21	SER
1	B	94	ILE
1	B	99	LYS
1	B	143	VAL
1	B	200	GLN
1	B	204	LEU
1	B	216	ASP
1	B	218	ILE
1	B	221	VAL
1	B	224	GLN
1	B	238	SER
1	B	277	MET
1	B	340	TYR
1	B	390	SER
1	B	402	SER
1	B	424	THR
1	B	428	VAL
1	B	436	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	HIS
1	A	275	ASN
1	B	224	GLN
1	B	289	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](#)

5 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	PPV	A	501	-	6,8,8	1.00	0	12,13,13	1.00	0
4	MOE	B	502	-	4,4,4	0.34	0	3,3,3	0.34	0
3	TOE	A	502	-	10,10,10	0.38	0	9,9,9	0.31	0
3	TOE	B	503	-	10,10,10	0.37	0	9,9,9	0.36	0
2	PPV	B	501	-	6,8,8	0.94	0	12,13,13	0.87	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
2	PPV	A	501	-	-	0/6/6/6	-
4	MOE	B	502	-	-	1/2/2/2	-
3	TOE	A	502	-	-	5/8/8/8	-
3	TOE	B	503	-	-	2/8/8/8	-
2	PPV	B	501	-	-	0/6/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	TOE	OC'-CD'-CE'-OF'
3	B	503	TOE	CH'-CG'-OF'-CE'
3	B	503	TOE	OC'-CD'-CE'-OF'
4	B	502	MOE	CA'-CB'-OC'-CD'
3	A	502	TOE	CH'-CG'-OF'-CE'
3	A	502	TOE	CA'-CB'-OC'-CD'
3	A	502	TOE	CD'-CE'-OF'-CG'
3	A	502	TOE	CG'-CH'-OI'-CK'

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PPV	1	0
4	B	502	MOE	1	0
3	A	502	TOE	1	0
3	B	503	TOE	4	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	418/441 (94%)	0.68	48 (11%)  	12, 54, 87, 106	3 (0%)
1	B	394/441 (89%)	0.76	53 (13%)  	25, 53, 84, 120	3 (0%)
All	All	812/882 (92%)	0.72	101 (12%)  	12, 54, 85, 120	6 (0%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	78	ASP	23.6
1	B	435	PRO	13.6
1	B	241	ASN	7.7
1	B	217	ALA	6.9
1	A	318	HIS	6.0
1	B	220	GLY	5.9
1	A	191	LEU	5.8
1	B	221	VAL	5.6
1	B	143	VAL	5.1
1	B	239	GLY	5.0
1	B	87	LEU	5.0
1	A	323	ILE	4.7
1	B	436	GLN	4.5
1	B	319	PHE	4.5
1	B	206	LEU	4.5
1	B	438	LEU	4.4
1	B	334	LEU	4.3
1	B	208	ASP	4.3
1	A	186	LEU	4.0
1	B	223	PRO	3.9
1	B	191	LEU	3.8
1	A	335	PRO	3.8
1	B	209	LEU	3.8
1	A	187	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	382	GLY	3.8
1	B	88	THR	3.7
1	A	184	ALA	3.6
1	B	145	GLY	3.6
1	B	211	VAL	3.6
1	B	345	PRO	3.6
1	B	174	ALA	3.6
1	A	438	LEU	3.5
1	A	331	THR	3.5
1	A	204	LEU	3.4
1	A	185	GLU	3.4
1	A	319	PHE	3.3
1	A	77	ALA	3.3
1	B	226	ALA	3.3
1	A	321	PRO	3.3
1	B	205	SER	3.3
1	A	334	LEU	3.3
1	A	174	ALA	3.2
1	A	324	MET	3.2
1	B	57	TYR	3.2
1	B	222	CYS	3.2
1	B	316	ALA	3.2
1	A	328	GLU	3.2
1	A	322	PRO	3.2
1	A	190	GLY	3.1
1	A	317	GLU	3.1
1	B	169	ALA	3.1
1	B	104	THR	3.1
1	A	420	THR	3.0
1	B	163[A]	ARG	3.0
1	B	437	MET	3.0
1	A	188	PRO	3.0
1	B	22	LEU	3.0
1	A	400	HIS	3.0
1	B	349	TYR	2.8
1	A	222	CYS	2.8
1	B	203	GLY	2.8
1	B	303	LEU	2.8
1	A	329	GLU	2.7
1	B	242	LEU	2.7
1	A	316	ALA	2.7
1	B	171	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	21	SER	2.7
1	B	281	GLY	2.7
1	A	433	SER	2.7
1	B	224	GLN	2.6
1	B	305	ASP	2.6
1	B	432	SER	2.6
1	B	150	TRP	2.6
1	A	203	GLY	2.6
1	A	209	LEU	2.6
1	B	202	VAL	2.6
1	A	310	ASP	2.6
1	A	332	LEU	2.5
1	A	241	ASN	2.5
1	A	172	ALA	2.5
1	B	398	GLY	2.5
1	B	347	ARG	2.5
1	B	214	LEU	2.5
1	A	105	LYS	2.5
1	B	439	TYR	2.4
1	A	320	SER	2.4
1	A	333	VAL	2.4
1	B	103	ALA	2.3
1	B	86	PRO	2.3
1	B	346	GLY	2.3
1	B	89	VAL	2.3
1	A	418	ASP	2.2
1	B	267	ARG	2.2
1	B	288	THR	2.2
1	A	325	ASP	2.1
1	A	23	LEU	2.1
1	A	57	TYR	2.1
1	A	397	HIS	2.0
1	A	14	LEU	2.0
1	A	40	ARG	2.0
1	A	417	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	TOE	B	503	11/11	0.79	0.27	20,20,20,20	0
4	MOE	B	502	5/5	0.87	0.23	20,20,20,20	0
3	TOE	A	502	11/11	0.90	0.26	20,20,20,20	0
2	PPV	B	501	9/9	0.91	0.09	53,58,77,80	0
2	PPV	A	501	9/9	0.93	0.11	45,51,85,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.