



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:36 PM UTC

PDB ID : 8WWE / pdb_00008wwe
Title : Crystal structure of (R)-DHPS dehydrogenase HpsN from Ruegeria pomeroyi DSS-3
Authors : Liu, L.; Tang, K.
Deposited on : 2023-10-25
Resolution : 2.90 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

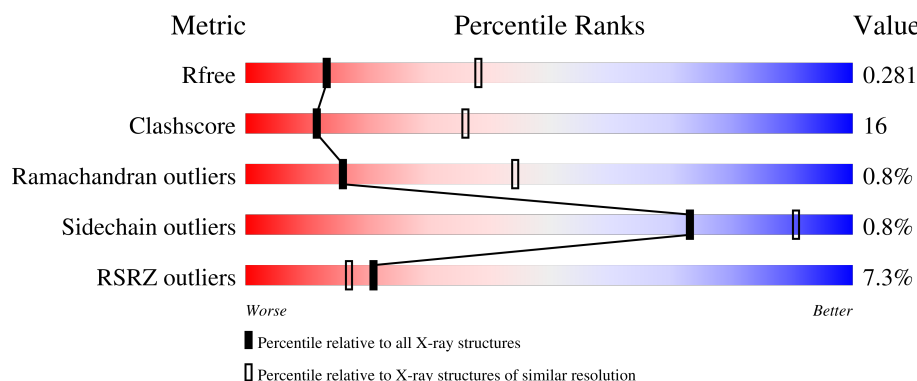
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	407	 4% 61% 28% 10%
1	B	407	 6% 65% 25% 9%
1	C	407	 8% 62% 25% 9%
1	D	407	 8% 63% 24% 11%

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
2	SO4	C	501	-	-	X	-

2 Entry composition [i](#)

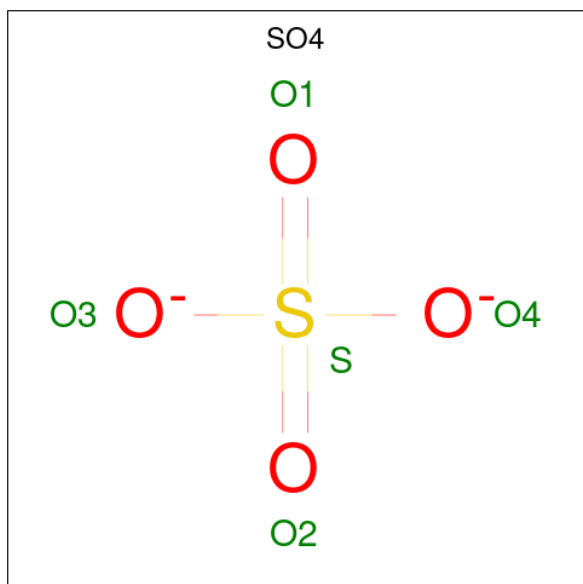
There are 2 unique types of molecules in this entry. The entry contains 11150 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (R)-DHPS dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2775	1754	475	530	16			
1	B	370	Total	C	N	O	S	0	0	0
			2811	1775	482	538	16			
1	C	369	Total	C	N	O	S	0	0	0
			2802	1771	481	533	17			
1	D	361	Total	C	N	O	S	0	0	0
			2737	1731	467	523	16			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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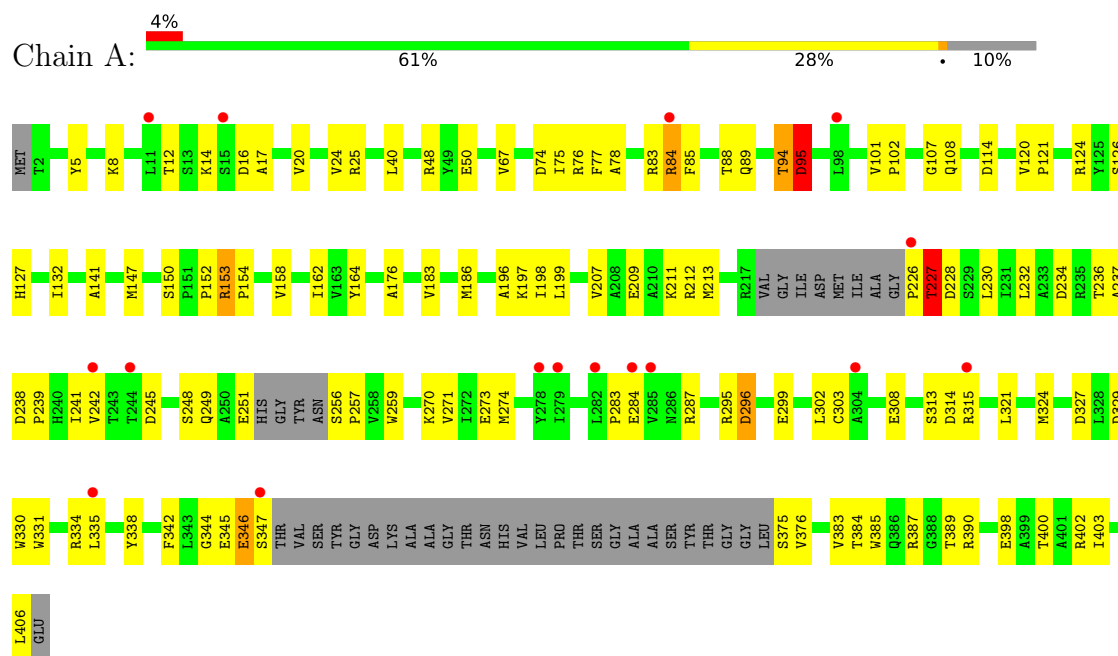
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

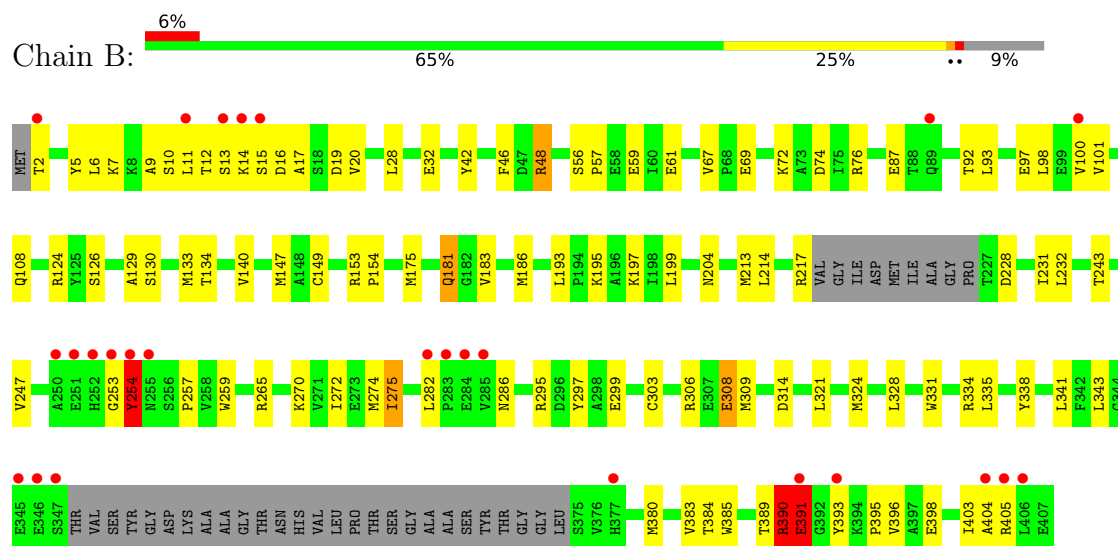
3 Residue-property plots

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

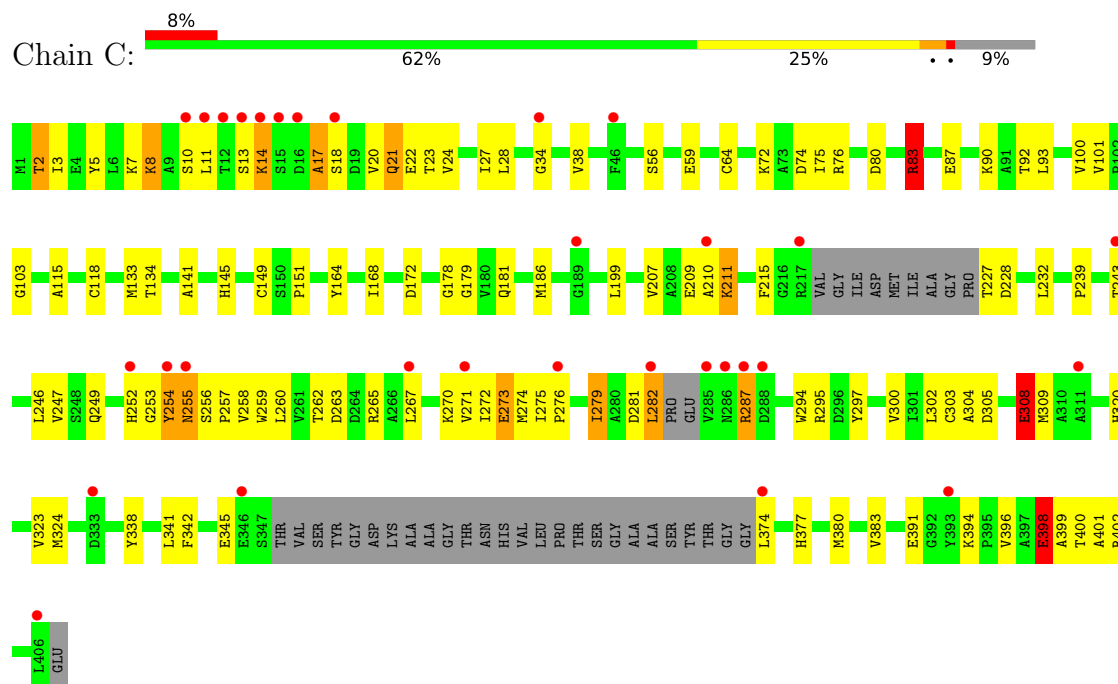
• Molecule 1: (R)-DHPS dehydrogenase



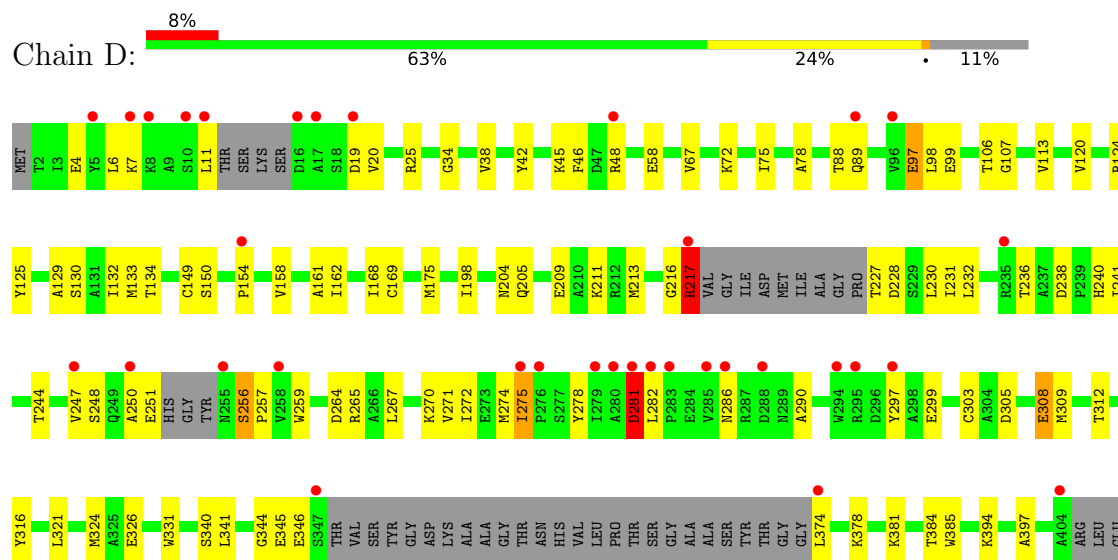
• Molecule 1: (R)-DHPS dehydrogenase



• Molecule 1: (R)-DHPS dehydrogenase



• Molecule 1: (R)-DHPS dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	68.05Å 122.86Å 210.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.20 – 2.90 46.20 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.20-2.90) 99.4 (46.20-2.90)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.242 , 0.280 0.245 , 0.281	Depositor DCC
R_{free} test set	1511 reflections (2.66%)	wwPDB-VP
Wilson B-factor (Å ²)	60.9	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.6	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	0.89	EDS
Total number of atoms	11150	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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: SO4

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	0.84	7/2826 (0.2%)	1.08	16/3837 (0.4%)
1	B	0.74	2/2864 (0.1%)	1.07	20/3890 (0.5%)
1	C	0.65	1/2853 (0.0%)	1.13	26/3872 (0.7%)
1	D	0.70	1/2786 (0.0%)	1.09	19/3783 (0.5%)
All	All	0.74	11/11329 (0.1%)	1.09	81/15382 (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	A	0	2
1	B	0	3
1	C	0	4
1	D	0	2
All	All	0	11

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	275	ILE	CA-CB	-21.94	1.43	1.54
1	D	275	ILE	CA-CB	18.54	1.64	1.54
1	A	84	ARG	CD-NE	17.15	1.70	1.46
1	A	67	VAL	CA-C	-12.65	1.43	1.53
1	A	84	ARG	NE-CZ	11.48	1.45	1.33
1	A	84	ARG	CZ-NH2	11.04	1.47	1.33
1	A	153	ARG	CD-NE	8.35	1.57	1.46
1	A	84	ARG	CG-CD	7.59	1.75	1.52
1	A	67	VAL	N-CA	6.97	1.51	1.46
1	C	287	ARG	CD-NE	5.32	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	48	ARG	CZ-NH1	5.21	1.40	1.32

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	ARG	CG-CD-NE	-20.55	66.79	112.00
1	B	390	ARG	CB-CG-CD	-19.10	67.37	111.30
1	D	217	ARG	NE-CZ-NH1	-15.82	105.68	121.50
1	D	217	ARG	CD-NE-CZ	12.86	142.40	124.40
1	B	48	ARG	CD-NE-CZ	-12.11	107.45	124.40
1	D	217	ARG	NE-CZ-NH2	11.76	129.79	119.20
1	C	83	ARG	CD-NE-CZ	-11.76	107.94	124.40
1	A	67	VAL	CA-C-O	10.29	125.22	119.15
1	C	398	GLU	CA-CB-CG	10.04	134.19	114.10
1	D	281	ASP	CA-C-N	-9.89	103.98	123.56
1	D	281	ASP	C-N-CA	-9.89	103.98	123.56
1	B	254	TYR	CB-CA-C	9.22	125.69	109.65
1	D	89	GLN	N-CA-CB	8.97	123.30	110.12
1	A	153	ARG	CB-CG-CD	8.95	131.89	111.30
1	A	153	ARG	NE-CZ-NH1	-8.85	112.65	121.50
1	B	391	GLU	N-CA-CB	-8.81	95.60	110.49
1	C	83	ARG	CG-CD-NE	8.74	131.23	112.00
1	C	287	ARG	CG-CD-NE	8.70	131.13	112.00
1	A	315	ARG	CG-CD-NE	8.62	130.97	112.00
1	B	254	TYR	N-CA-CB	-8.52	97.83	110.53
1	C	14	LYS	CD-CE-NZ	8.49	139.07	111.90
1	D	89	GLN	CA-CB-CG	8.46	131.03	114.10
1	C	308	GLU	CA-CB-CG	8.29	130.67	114.10
1	C	21	GLN	CA-CB-CG	-8.18	97.74	114.10
1	A	84	ARG	NE-CZ-NH1	7.86	129.36	121.50
1	A	67	VAL	O-C-N	-7.85	114.74	121.57
1	A	346	GLU	CA-CB-CG	-7.67	98.77	114.10
1	B	48	ARG	CA-CB-CG	7.62	129.34	114.10
1	B	48	ARG	CG-CD-NE	7.55	128.61	112.00
1	B	391	GLU	CB-CA-C	7.54	125.42	110.42
1	C	398	GLU	N-CA-CB	7.52	120.91	110.01
1	D	308	GLU	CB-CA-C	-7.47	98.86	110.81
1	C	8	LYS	CA-CB-CG	7.30	128.70	114.10
1	C	398	GLU	CB-CG-CD	7.21	124.86	112.60
1	D	89	GLN	CB-CA-C	-7.18	98.86	110.79
1	A	84	ARG	CD-NE-CZ	-7.17	114.37	124.40
1	C	10	SER	CB-CA-C	7.14	123.56	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	308	GLU	CB-CG-CD	-7.07	100.57	112.60
1	B	390	ARG	CA-CB-CG	7.01	128.12	114.10
1	A	153	ARG	NE-CZ-NH2	6.95	125.46	119.20
1	C	294	TRP	CA-C-N	-6.80	111.33	122.54
1	C	294	TRP	C-N-CA	-6.80	111.33	122.54
1	C	287	ARG	CA-CB-CG	6.73	127.55	114.10
1	B	133	MET	N-CA-CB	-6.72	98.30	109.72
1	C	10	SER	N-CA-CB	-6.66	100.20	110.46
1	A	84	ARG	NH1-CZ-NH2	-6.64	110.67	119.30
1	A	346	GLU	N-CA-C	-6.55	103.41	111.40
1	A	50	GLU	N-CA-CB	-6.32	102.38	111.54
1	C	308	GLU	N-CA-CB	-6.16	99.75	109.78
1	B	391	GLU	CA-C-N	6.14	133.44	121.41
1	B	391	GLU	C-N-CA	6.14	133.44	121.41
1	D	217	ARG	CB-CA-C	6.04	121.58	110.10
1	D	88	THR	CA-C-N	-6.01	112.23	120.28
1	D	88	THR	C-N-CA	-6.01	112.23	120.28
1	D	265	ARG	CA-CB-CG	5.96	126.02	114.10
1	C	83	ARG	NE-CZ-NH2	-5.88	113.91	119.20
1	C	14	LYS	CA-CB-CG	5.81	125.72	114.10
1	C	398	GLU	CB-CA-C	-5.78	101.80	110.88
1	B	254	TYR	CB-CG-CD2	-5.76	112.15	120.80
1	A	153	ARG	CB-CA-C	5.75	117.64	109.08
1	C	254	TYR	N-CA-C	-5.71	99.88	108.96
1	D	97	GLU	CA-C-N	-5.69	113.97	122.39
1	D	97	GLU	C-N-CA	-5.69	113.97	122.39
1	C	295	ARG	NE-CZ-NH2	-5.68	114.09	119.20
1	B	133	MET	CG-SD-CE	-5.60	88.57	100.90
1	B	391	GLU	CB-CG-CD	5.53	122.00	112.60
1	D	264	ASP	CA-C-N	5.50	127.96	120.54
1	D	264	ASP	C-N-CA	5.50	127.96	120.54
1	C	83	ARG	N-CA-C	-5.49	104.94	111.69
1	C	308	GLU	CB-CA-C	5.48	119.84	110.74
1	A	296	ASP	CB-CA-C	5.45	118.78	109.24
1	B	48	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	D	275	ILE	CB-CA-C	-5.32	107.03	114.00
1	B	48	ARG	NE-CZ-NH1	-5.27	116.23	121.50
1	A	95	ASP	N-CA-CB	-5.21	101.68	110.49
1	D	217	ARG	CB-CG-CD	5.13	123.11	111.30
1	B	391	GLU	CA-CB-CG	5.07	124.24	114.10
1	C	279	ILE	N-CA-CB	5.07	117.44	110.54
1	C	295	ARG	CB-CG-CD	5.04	122.89	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	181	GLN	CA-C-N	5.02	125.41	119.94
1	B	181	GLN	C-N-CA	5.02	125.41	119.94

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	227	THR	Peptide
1	A	94	THR	Peptide
1	B	15	SER	Peptide
1	B	254	TYR	Sidechain
1	B	390	ARG	Peptide
1	C	13	SER	Peptide
1	C	2	THR	Peptide
1	C	273	GLU	Sidechain
1	C	398	GLU	Sidechain
1	D	217	ARG	Sidechain
1	D	374	LEU	Peptide

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	2775	0	2774	103	0
1	B	2811	0	2798	90	0
1	C	2802	0	2801	110	0
1	D	2737	0	2728	92	0
2	B	10	0	0	1	0
2	C	10	0	0	0	7
2	D	5	0	0	0	0
All	All	11150	0	11101	353	7

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 16.

All (353) 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:84:ARG:CD	1:A:84:ARG:CG	1.75	1.64
1:A:84:ARG:CD	1:A:84:ARG:NE	1.70	1.50
1:A:308:GLU:OE2	1:B:2:THR:OG1	1.67	1.11
1:B:149:CYS:HB3	1:B:175:MET:HE3	1.42	1.01
1:C:282:LEU:H	1:C:287:ARG:HE	1.10	0.99
1:C:64:CYS:HG	1:C:164:TYR:HD1	1.15	0.89
1:B:67:VAL:O	1:B:72:LYS:NZ	2.08	0.87
1:C:80:ASP:HA	1:C:83:ARG:HH22	1.39	0.86
1:C:304:ALA:N	1:C:308:GLU:OE1	2.08	0.85
1:D:303:CYS:HB3	1:D:308:GLU:HG2	1.59	0.85
1:B:331:TRP:HE3	1:B:335:LEU:HD11	1.44	0.82
1:C:101:VAL:HG22	1:C:398:GLU:OE1	1.81	0.80
1:C:282:LEU:N	1:C:287:ARG:HE	1.79	0.79
1:C:20:VAL:O	1:C:23:THR:OG1	2.01	0.79
1:A:238:ASP:HB3	1:A:241:ILE:HD12	1.66	0.78
1:B:186:MET:HE3	1:B:199:LEU:HD11	1.67	0.77
1:A:153:ARG:HG2	1:A:154:PRO:HD2	1.67	0.76
1:A:25:ARG:NE	1:B:32:GLU:OE2	2.18	0.76
1:B:270:LYS:O	1:B:274:MET:HG3	1.87	0.75
1:B:254:TYR:HD1	1:B:254:TYR:H	1.32	0.75
1:A:84:ARG:CD	1:A:84:ARG:CZ	2.65	0.75
1:C:210:ALA:O	1:C:211:LYS:HB2	1.86	0.74
1:B:175:MET:HE1	1:B:186:MET:HG2	1.70	0.72
1:C:267:LEU:O	1:C:271:VAL:HG23	1.89	0.72
1:A:83:ARG:NH2	1:A:84:ARG:HG2	2.05	0.72
1:A:199:LEU:HD23	1:A:211:LYS:HG2	1.70	0.71
1:C:179:GLY:HA2	1:C:207:VAL:HG22	1.72	0.71
1:C:72:LYS:O	1:C:76:ARG:HG3	1.91	0.70
1:D:303:CYS:CB	1:D:308:GLU:HG2	2.21	0.69
1:C:270:LYS:HG2	1:C:274:MET:HE2	1.73	0.69
1:A:346:GLU:HB3	1:A:389:THR:HG23	1.74	0.69
1:C:80:ASP:HA	1:C:83:ARG:NH2	2.07	0.69
1:C:5:TYR:HB3	1:C:7:LYS:O	1.93	0.69
1:A:108:GLN:HG2	1:A:384:THR:HG22	1.75	0.68
1:C:103:GLY:HA3	1:C:391:GLU:HG3	1.73	0.68
1:C:272:ILE:HD11	1:D:7:LYS:HB2	1.75	0.68
1:D:75:ILE:HG23	1:D:132:ILE:HD11	1.76	0.68
1:B:390:ARG:NH2	1:B:398:GLU:OE2	2.26	0.68
1:C:282:LEU:H	1:C:287:ARG:NE	1.88	0.68
1:C:228:ASP:HB3	1:C:259:TRP:HZ3	1.60	0.67
1:B:98:LEU:HD23	1:B:100:VAL:HG23	1.76	0.67
1:C:227:THR:HG21	1:C:252:HIS:HE1	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:CYS:HB3	1:B:308:GLU:HB3	1.76	0.66
1:D:303:CYS:HB3	1:D:308:GLU:CG	2.25	0.66
1:A:124:ARG:HH11	1:A:126:SER:HB3	1.59	0.66
1:C:255:ASN:OD1	1:D:204:ASN:HB2	1.95	0.66
1:A:75:ILE:HG23	1:A:132:ILE:HD11	1.76	0.66
1:D:238:ASP:HB3	1:D:241:ILE:CD1	2.25	0.66
1:A:152:PRO:HG3	1:A:176:ALA:HB1	1.78	0.66
1:D:19:ASP:OD1	1:D:20:VAL:N	2.28	0.65
1:C:18:SER:N	1:C:22:GLU:OE1	2.28	0.65
1:B:147:MET:HE3	1:B:193:LEU:HB3	1.79	0.65
1:D:272:ILE:HA	1:D:275:ILE:HD11	1.78	0.65
1:A:101:VAL:HG12	1:A:398:GLU:HG2	1.79	0.64
1:B:124:ARG:HH11	1:B:126:SER:H	1.44	0.64
1:A:124:ARG:NH1	1:A:126:SER:HB3	2.12	0.64
1:C:297:TYR:CE1	1:D:11:LEU:HD12	2.32	0.64
1:D:198:ILE:HD11	1:D:378:LYS:HG3	1.77	0.64
1:C:243:THR:O	1:C:247:VAL:HG23	1.97	0.64
1:C:255:ASN:OD1	1:D:205:GLN:N	2.30	0.63
1:D:257:PRO:HA	1:D:297:TYR:HB3	1.78	0.63
1:C:270:LYS:O	1:C:273:GLU:HB3	1.98	0.63
1:D:42:TYR:HD1	1:D:46:PHE:HE2	1.46	0.63
1:D:124:ARG:NH1	1:D:125:TYR:HB2	2.14	0.63
1:C:262:THR:O	1:C:303:CYS:N	2.32	0.63
1:A:284:GLU:HA	1:A:287:ARG:HD2	1.80	0.63
1:B:228:ASP:HB2	1:B:259:TRP:HZ3	1.62	0.63
1:A:89:GLN:HE22	1:A:375:SER:HB2	1.63	0.62
1:B:149:CYS:HB3	1:B:175:MET:CE	2.26	0.62
1:B:153:ARG:HG3	1:B:154:PRO:HD2	1.81	0.62
1:A:270:LYS:O	1:A:273:GLU:HG2	2.00	0.61
1:C:303:CYS:HB3	1:C:308:GLU:OE1	2.00	0.61
1:A:321:LEU:HD21	1:A:335:LEU:HD13	1.82	0.61
1:D:45:LYS:HE2	1:D:46:PHE:CE1	2.35	0.61
1:B:87:GLU:HG3	1:B:140:VAL:HG13	1.82	0.61
1:D:6:LEU:N	1:D:6:LEU:HD12	2.15	0.61
1:C:265:ARG:NH2	1:D:4:GLU:OE2	2.34	0.61
1:C:239:PRO:HB3	1:C:274:MET:HE1	1.83	0.61
1:D:275:ILE:HD12	1:D:275:ILE:H	1.65	0.61
1:A:83:ARG:HH22	1:A:84:ARG:HG2	1.64	0.61
1:A:390:ARG:NH1	1:A:398:GLU:OE2	2.34	0.60
1:B:254:TYR:CD1	1:B:254:TYR:N	2.61	0.60
1:C:239:PRO:CB	1:C:274:MET:HE1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ILE:HG22	1:C:168:ILE:HD11	1.83	0.59
1:B:321:LEU:HD21	1:B:335:LEU:CD2	2.32	0.59
1:D:267:LEU:O	1:D:271:VAL:HG23	2.03	0.59
1:C:83:ARG:O	1:C:87:GLU:HG3	2.03	0.59
1:D:270:LYS:O	1:D:274:MET:HG3	2.01	0.59
1:C:275:ILE:HG13	1:C:279:ILE:HD11	1.86	0.58
1:C:56:SER:OG	1:C:59:GLU:HG3	2.03	0.58
1:D:25:ARG:HG3	1:D:213:MET:HE1	1.85	0.58
1:A:302:LEU:HB2	1:B:6:LEU:HD11	1.85	0.58
1:C:276:PRO:HA	1:C:279:ILE:HD12	1.86	0.58
1:D:232:LEU:HD12	1:D:321:LEU:HD11	1.86	0.58
1:D:244:THR:O	1:D:247:VAL:HG12	2.03	0.57
1:D:282:LEU:HB3	1:D:286:ASN:HB2	1.85	0.57
1:B:175:MET:HE1	1:B:186:MET:CG	2.34	0.57
1:D:130:SER:O	1:D:134:THR:HG23	2.04	0.57
1:A:120:VAL:HG11	1:A:162:ILE:HD12	1.87	0.57
1:B:57:PRO:O	1:B:61:GLU:HG2	2.05	0.57
1:C:93:LEU:HD11	1:C:377:HIS:CD2	2.40	0.57
1:A:232:LEU:HD11	1:A:313:SER:HB2	1.86	0.56
1:B:321:LEU:HD21	1:B:335:LEU:HD22	1.87	0.56
1:D:120:VAL:HG11	1:D:162:ILE:HD12	1.87	0.56
1:A:232:LEU:HD13	1:A:321:LEU:HD11	1.88	0.56
1:A:230:LEU:HD21	1:A:232:LEU:HD12	1.88	0.56
1:C:14:LYS:HA	1:C:17:ALA:O	2.06	0.55
1:C:272:ILE:O	1:C:275:ILE:HG22	2.07	0.55
1:C:302:LEU:CB	1:D:6:LEU:HD11	2.37	0.55
1:C:303:CYS:CB	1:C:308:GLU:OE1	2.55	0.55
1:D:34:GLY:HA3	1:D:38:VAL:HG21	1.89	0.55
1:B:56:SER:OG	1:B:59:GLU:HG3	2.07	0.55
1:C:305:ASP:OD1	1:C:308:GLU:HB2	2.07	0.55
1:C:247:VAL:CG1	1:C:282:LEU:HD11	2.37	0.54
1:B:195:LYS:O	1:B:197:LYS:NZ	2.41	0.54
1:D:236:THR:HG21	1:D:326:GLU:HG3	1.89	0.54
1:A:5:TYR:OH	1:A:14:LYS:HB3	2.08	0.53
1:B:389:THR:O	1:B:391:GLU:HB2	2.08	0.53
1:B:389:THR:O	1:B:391:GLU:HG3	2.08	0.53
1:C:11:LEU:HD11	1:D:297:TYR:CE1	2.43	0.53
1:A:20:VAL:O	1:A:24:VAL:HG23	2.08	0.53
1:B:92:THR:HB	1:C:92:THR:HG22	1.90	0.53
1:D:34:GLY:HA3	1:D:38:VAL:CG2	2.39	0.53
1:D:309:MET:HE3	1:D:331:TRP:CH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:THR:HG21	1:D:78:ALA:HB1	1.90	0.53
1:D:303:CYS:HB2	1:D:309:MET:HG2	1.90	0.53
1:D:124:ARG:HH12	1:D:125:TYR:HB2	1.74	0.53
1:A:338:TYR:CE1	1:A:383:VAL:HB	2.44	0.53
1:B:149:CYS:SG	1:B:186:MET:HE2	2.49	0.53
1:C:399:ALA:HA	1:C:402:ARG:HD2	1.91	0.53
1:C:279:ILE:O	1:C:282:LEU:HD22	2.08	0.52
1:C:249:GLN:O	1:C:253:GLY:HA3	2.09	0.52
1:A:329:ASP:OD1	1:A:387:ARG:NH1	2.33	0.52
1:A:84:ARG:HD3	1:A:84:ARG:HH21	1.75	0.52
1:D:209:GLU:C	1:D:211:LYS:H	2.17	0.52
1:A:403:ILE:CG2	1:D:133:MET:HE3	2.40	0.52
1:B:331:TRP:CE3	1:B:335:LEU:HD11	2.35	0.52
1:B:282:LEU:HD13	1:B:286:ASN:HB2	1.91	0.52
1:A:295:ARG:HH12	1:B:48:ARG:NH1	2.08	0.52
1:B:9:ALA:HB3	1:B:12:THR:HB	1.92	0.52
1:A:400:THR:HG22	1:D:129:ALA:HA	1.92	0.52
1:B:328:LEU:HD22	1:B:343:LEU:HB3	1.92	0.52
1:C:275:ILE:O	1:C:279:ILE:HD12	2.10	0.51
1:D:67:VAL:HG23	1:D:72:LYS:HE3	1.91	0.51
1:D:303:CYS:HB3	1:D:308:GLU:HB3	1.92	0.51
1:C:2:THR:HG23	1:C:3:ILE:HA	1.93	0.51
1:C:7:LYS:HG2	1:C:8:LYS:H	1.74	0.51
1:A:402:ARG:HG2	1:A:406:LEU:HD12	1.92	0.51
1:C:282:LEU:N	1:C:287:ARG:HH21	2.08	0.51
1:D:309:MET:HE3	1:D:331:TRP:HH2	1.76	0.51
1:A:84:ARG:CD	1:A:84:ARG:CB	2.81	0.51
1:A:303:CYS:HA	1:A:308:GLU:OE1	2.11	0.51
1:A:283:PRO:O	1:A:287:ARG:HG3	2.11	0.51
1:C:14:LYS:HD2	1:C:18:SER:HA	1.92	0.51
1:A:183:VAL:HG13	1:A:199:LEU:HD22	1.93	0.50
1:A:314:ASP:OD2	1:A:334:ARG:NH1	2.43	0.50
1:A:239:PRO:HG2	1:A:270:LYS:NZ	2.26	0.50
1:A:302:LEU:HD12	1:A:303:CYS:H	1.77	0.50
1:B:396:VAL:HB	1:C:74:ASP:CG	2.36	0.50
1:C:320:HIS:CE1	1:C:342:PHE:HE2	2.29	0.50
1:D:58:GLU:CD	1:D:58:GLU:H	2.19	0.50
1:B:338:TYR:CE1	1:B:383:VAL:HB	2.46	0.50
1:C:199:LEU:HD23	1:C:215:PHE:CE2	2.46	0.50
1:D:238:ASP:HB3	1:D:241:ILE:HD12	1.91	0.50
1:B:181:GLN:H	1:B:181:GLN:CD	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:THR:O	1:B:247:VAL:HG23	2.11	0.50
1:A:150:SER:HB3	1:A:158:VAL:HG13	1.92	0.50
1:A:107:GLY:HA3	1:A:385:TRP:NE1	2.26	0.50
1:C:302:LEU:HB2	1:D:6:LEU:HD11	1.92	0.50
1:D:281:ASP:O	1:D:282:LEU:HD23	2.12	0.50
1:A:83:ARG:HH22	1:A:84:ARG:CG	2.25	0.50
1:B:98:LEU:HD23	1:B:100:VAL:CG2	2.41	0.50
1:C:118:CYS:SG	1:C:134:THR:HG22	2.52	0.50
1:C:320:HIS:CE1	1:C:342:PHE:CE2	3.00	0.50
1:C:247:VAL:HG12	1:C:282:LEU:HD11	1.94	0.49
1:C:276:PRO:HA	1:C:279:ILE:CD1	2.41	0.49
1:A:124:ARG:HD3	1:A:126:SER:H	1.76	0.49
1:B:306:ARG:O	1:B:309:MET:HB2	2.12	0.49
1:C:34:GLY:HA3	1:C:38:VAL:CG2	2.42	0.49
1:A:141:ALA:HB2	1:A:376:VAL:HG13	1.95	0.49
1:C:257:PRO:HD3	1:D:205:GLN:NE2	2.26	0.49
1:D:42:TYR:CD1	1:D:46:PHE:HE2	2.29	0.49
1:A:234:ASP:OD1	1:A:236:THR:OG1	2.27	0.49
1:C:257:PRO:HA	1:C:297:TYR:HB3	1.95	0.49
1:C:115:ALA:HA	1:C:145:HIS:O	2.13	0.49
1:C:338:TYR:CE1	1:C:383:VAL:HB	2.48	0.49
1:D:98:LEU:N	1:D:106:THR:O	2.44	0.49
1:D:312:THR:HG23	1:D:316:TYR:HE1	1.78	0.49
1:D:11:LEU:HD22	1:D:46:PHE:CD1	2.49	0.48
1:A:324:MET:HG2	1:A:345:GLU:HG2	1.94	0.48
1:B:183:VAL:HG22	1:B:199:LEU:HD21	1.95	0.48
1:B:14:LYS:HA	1:B:17:ALA:O	2.12	0.48
1:C:282:LEU:C	1:C:287:ARG:HH21	2.21	0.48
1:A:198:ILE:HD12	1:A:199:LEU:H	1.76	0.48
1:A:327:ASP:OD2	1:A:330:TRP:HB2	2.13	0.48
1:C:8:LYS:HA	1:D:299:GLU:HG3	1.95	0.48
1:C:34:GLY:HA3	1:C:38:VAL:HG21	1.95	0.48
1:A:83:ARG:NH2	1:A:84:ARG:CG	2.77	0.48
1:A:299:GLU:CD	1:B:13:SER:HA	2.38	0.48
1:B:11:LEU:HD12	1:B:16:ASP:OD2	2.14	0.48
1:A:213:MET:SD	1:B:213:MET:HE1	2.54	0.48
1:B:42:TYR:HD1	1:B:46:PHE:CE1	2.32	0.47
1:B:231:ILE:HG21	1:B:324:MET:HE3	1.96	0.47
1:B:257:PRO:HA	1:B:297:TYR:HB3	1.96	0.47
1:B:108:GLN:HG2	1:B:384:THR:HG22	1.96	0.47
1:B:124:ARG:NH1	1:B:126:SER:HB3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:GLU:H	1:A:346:GLU:HG3	1.37	0.47
1:B:405:ARG:HH12	1:C:374:LEU:HD12	1.80	0.47
1:A:121:PRO:HG2	1:A:127:HIS:CE1	2.50	0.47
1:D:228:ASP:HB2	1:D:259:TRP:HZ3	1.79	0.47
1:B:14:LYS:C	1:B:16:ASP:H	2.23	0.47
1:B:254:TYR:HD1	1:B:254:TYR:N	2.04	0.47
1:B:403:ILE:HG21	1:C:133:MET:HE1	1.97	0.47
1:D:48:ARG:O	1:D:154:PRO:HG3	2.15	0.47
1:A:342:PHE:HB3	1:A:347:SER:HB2	1.96	0.47
1:A:12:THR:HG21	1:B:257:PRO:HG3	1.97	0.47
1:C:273:GLU:O	1:C:276:PRO:HD2	2.15	0.47
1:A:403:ILE:HG22	1:D:133:MET:HE3	1.97	0.47
1:D:248:SER:O	1:D:251:GLU:HG2	2.15	0.47
1:B:393:TYR:CE2	1:B:395:PRO:HG3	2.50	0.46
1:B:403:ILE:C	1:B:405:ARG:H	2.23	0.46
1:C:8:LYS:HA	1:D:299:GLU:OE1	2.15	0.46
1:C:303:CYS:CA	1:C:308:GLU:OE1	2.63	0.46
1:C:324:MET:HG2	1:C:345:GLU:HG2	1.95	0.46
1:D:216:GLY:O	1:D:217:ARG:HB3	2.15	0.46
1:C:23:THR:O	1:C:27:ILE:HG13	2.14	0.46
1:C:141:ALA:O	1:C:380:MET:HE3	2.16	0.46
1:A:237:ALA:O	1:A:239:PRO:HD3	2.15	0.46
1:B:19:ASP:OD2	1:B:20:VAL:N	2.49	0.46
1:B:341:LEU:HD21	1:B:343:LEU:HD21	1.98	0.46
1:C:282:LEU:N	1:C:287:ARG:NE	2.55	0.46
1:C:302:LEU:HG	1:C:303:CYS:N	2.28	0.46
1:A:48:ARG:HH22	1:B:295:ARG:HD3	1.81	0.46
1:A:245:ASP:O	1:A:249:GLN:NE2	2.49	0.46
1:B:69:GLU:OE2	1:B:76:ARG:NH2	2.48	0.46
1:C:207:VAL:O	1:C:210:ALA:O	2.34	0.46
1:C:151:PRO:HB3	1:C:178:GLY:HA3	1.97	0.45
1:C:260:LEU:HD23	1:C:300:VAL:HG13	1.98	0.45
1:A:232:LEU:HD23	1:A:331:TRP:CZ3	2.52	0.45
1:C:263:ASP:HA	1:C:303:CYS:O	2.17	0.45
1:A:107:GLY:HA3	1:A:385:TRP:CE2	2.51	0.45
1:A:186:MET:HE3	1:A:199:LEU:HD11	1.98	0.45
1:B:129:ALA:HB1	1:C:400:THR:HA	1.98	0.45
1:A:239:PRO:HB2	1:A:274:MET:HE1	1.98	0.45
1:B:11:LEU:HA	1:B:16:ASP:OD2	2.17	0.45
1:B:130:SER:O	1:B:134:THR:HG23	2.17	0.45
1:C:323:VAL:HG23	1:C:341:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:HB2	1:B:6:LEU:CD1	2.47	0.45
1:C:302:LEU:HB3	1:D:6:LEU:HD11	1.99	0.45
1:D:250:ALA:HB2	1:D:290:ALA:HA	1.99	0.45
1:B:265:ARG:NH2	2:B:501:SO4:O1	2.49	0.45
1:C:24:VAL:CG1	1:C:210:ALA:HB2	2.47	0.45
1:C:255:ASN:HB3	1:C:256:SER:H	1.61	0.44
1:A:83:ARG:CZ	1:A:84:ARG:HG2	2.47	0.44
1:A:76:ARG:NH1	1:A:164:TYR:OH	2.50	0.44
1:D:230:LEU:HD22	1:D:321:LEU:CD1	2.47	0.44
1:B:97:GLU:HG2	1:B:385:TRP:HZ2	1.82	0.44
1:B:93:LEU:HD12	1:B:380:MET:HE1	1.99	0.44
1:A:85:PHE:O	1:A:88:THR:HB	2.18	0.44
1:A:152:PRO:HG3	1:A:176:ALA:C	2.42	0.44
1:A:186:MET:CE	1:A:199:LEU:HD11	2.48	0.44
1:A:257:PRO:HB2	1:A:259:TRP:CH2	2.53	0.44
1:A:259:TRP:HE1	1:A:299:GLU:CD	2.25	0.44
1:B:282:LEU:HD13	1:B:286:ASN:CB	2.47	0.44
1:C:17:ALA:HB3	1:C:23:THR:HG23	2.00	0.44
1:C:83:ARG:HH21	1:C:83:ARG:HD2	1.13	0.44
1:B:124:ARG:HD3	1:B:126:SER:H	1.82	0.43
1:A:14:LYS:C	1:A:16:ASP:H	2.27	0.43
1:A:74:ASP:OD1	1:D:394:LYS:HB3	2.18	0.43
1:A:226:PRO:O	1:A:228:ASP:N	2.51	0.43
1:B:314:ASP:OD2	1:B:334:ARG:NH1	2.46	0.43
1:D:230:LEU:HD23	1:D:231:ILE:C	2.43	0.43
1:B:28:LEU:HD22	1:B:214:LEU:HD11	2.01	0.43
1:C:21:GLN:HG3	1:C:209:GLU:HG2	2.00	0.43
1:D:67:VAL:HG11	1:D:161:ALA:HA	2.00	0.43
1:C:270:LYS:CG	1:C:274:MET:HE2	2.46	0.43
1:D:324:MET:HG2	1:D:345:GLU:HG3	2.00	0.43
1:C:232:LEU:HD22	1:C:309:MET:HB3	2.00	0.43
1:D:381:LYS:HE2	1:D:381:LYS:HB3	1.81	0.43
1:A:147:MET:HE3	1:A:147:MET:HB2	1.93	0.43
1:B:390:ARG:CA	1:B:391:GLU:HB2	2.47	0.42
1:C:90:LYS:NZ	1:C:380:MET:HE1	2.34	0.42
1:D:45:LYS:O	1:D:48:ARG:HD2	2.18	0.42
1:D:97:GLU:HA	1:D:107:GLY:HA2	2.01	0.42
1:D:274:MET:HE2	1:D:278:TYR:CE1	2.54	0.42
1:A:8:LYS:HA	1:B:299:GLU:HG2	2.01	0.42
1:A:248:SER:HA	1:A:251:GLU:CG	2.50	0.42
1:B:5:TYR:OH	1:B:14:LYS:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:HD23	1:A:40:LEU:HA	1.88	0.42
1:B:232:LEU:HD11	1:B:335:LEU:HD21	2.01	0.42
1:C:100:VAL:HG23	1:C:401:ALA:HB1	2.02	0.42
1:C:255:ASN:HD22	1:C:255:ASN:HA	1.55	0.42
1:D:230:LEU:HD22	1:D:321:LEU:HD12	2.01	0.42
1:D:303:CYS:CA	1:D:308:GLU:HG2	2.49	0.42
1:D:344:GLY:C	1:D:346:GLU:H	2.26	0.42
1:A:295:ARG:HA	1:B:7:LYS:NZ	2.34	0.42
1:D:227:THR:HG22	1:D:228:ASP:H	1.85	0.42
1:D:303:CYS:HB3	1:D:308:GLU:CB	2.49	0.42
1:A:77:PHE:CZ	1:D:99:GLU:HG2	2.55	0.42
1:B:390:ARG:NH2	1:B:398:GLU:CD	2.78	0.42
1:A:74:ASP:HA	1:D:394:LYS:HD3	2.01	0.42
1:A:242:VAL:CG2	1:A:271:VAL:HG21	2.50	0.42
1:C:246:LEU:HD22	1:C:258:VAL:HG21	2.01	0.42
1:A:147:MET:HE1	1:A:196:ALA:HB2	2.01	0.42
1:D:113:VAL:HG21	1:D:198:ILE:HG22	2.02	0.42
1:B:74:ASP:CG	1:C:396:VAL:HB	2.44	0.42
1:A:78:ALA:HB2	1:D:397:ALA:HA	2.02	0.42
1:A:209:GLU:HG3	1:A:213:MET:HE3	2.01	0.42
1:A:227:THR:O	1:A:256:SER:HB3	2.20	0.42
1:D:58:GLU:CD	1:D:58:GLU:N	2.77	0.42
1:A:295:ARG:HG3	1:A:296:ASP:N	2.33	0.41
1:D:107:GLY:HA3	1:D:385:TRP:CE2	2.55	0.41
1:D:321:LEU:HD23	1:D:341:LEU:HD13	2.01	0.41
1:C:255:ASN:HA	1:C:297:TYR:CZ	2.54	0.41
1:D:209:GLU:C	1:D:211:LYS:N	2.78	0.41
1:A:114:ASP:HB2	1:A:197:LYS:HZ3	1.85	0.41
1:A:259:TRP:CD1	1:A:299:GLU:HB2	2.55	0.41
1:C:24:VAL:HG13	1:C:210:ALA:HB2	2.02	0.41
1:C:281:ASP:C	1:C:287:ARG:HH21	2.29	0.41
1:D:240:HIS:HD2	1:D:278:TYR:OH	2.04	0.41
1:C:145:HIS:HA	1:C:172:ASP:OD2	2.21	0.41
1:A:238:ASP:OD1	1:A:238:ASP:C	2.63	0.41
1:A:101:VAL:O	1:A:102:PRO:C	2.64	0.41
1:C:5:TYR:HB2	1:C:8:LYS:HE2	2.03	0.41
1:C:149:CYS:SG	1:C:186:MET:HE2	2.61	0.41
1:C:181:GLN:H	1:C:181:GLN:CD	2.27	0.41
1:C:338:TYR:O	1:C:383:VAL:HG12	2.21	0.41
1:A:327:ASP:CG	1:A:330:TRP:HB2	2.45	0.41
1:C:24:VAL:O	1:C:28:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:VAL:CG2	1:C:401:ALA:HB1	2.50	0.41
1:D:149:CYS:CB	1:D:175:MET:HB2	2.51	0.41
1:D:227:THR:O	1:D:256:SER:OG	2.38	0.41
1:A:77:PHE:HZ	1:D:99:GLU:CG	2.34	0.40
1:A:344:GLY:C	1:A:346:GLU:H	2.29	0.40
1:D:150:SER:HB3	1:D:158:VAL:HG13	2.04	0.40
1:D:305:ASP:OD1	1:D:305:ASP:N	2.54	0.40
1:A:77:PHE:HZ	1:D:99:GLU:HG2	1.86	0.40
1:A:94:THR:HG22	1:A:95:ASP:O	2.21	0.40
1:A:212:ARG:CD	1:B:217:ARG:HB2	2.51	0.40
1:B:14:LYS:HA	1:B:14:LYS:HD2	1.96	0.40
1:B:181:GLN:OE1	1:B:181:GLN:N	2.39	0.40
1:B:11:LEU:HD12	1:B:16:ASP:CG	2.46	0.40
1:B:74:ASP:HA	1:C:394:LYS:HD3	2.03	0.40
1:B:100:VAL:HG12	1:B:101:VAL:HG23	2.03	0.40
1:B:124:ARG:HH11	1:B:126:SER:HB3	1.87	0.40
1:B:147:MET:CE	1:B:193:LEU:HD13	2.52	0.40
1:B:214:LEU:HD23	1:B:214:LEU:HA	1.96	0.40
1:A:207:VAL:O	1:A:211:LYS:HG3	2.22	0.40
1:C:255:ASN:CG	1:D:204:ASN:HB2	2.46	0.40
1:B:272:ILE:O	1:B:275:ILE:HG22	2.21	0.40
1:C:324:MET:CG	1:C:345:GLU:HG2	2.51	0.40
1:D:168:ILE:HG13	1:D:169:CYS:N	2.35	0.40
1:D:340:SER:HA	1:D:384:THR:O	2.22	0.40

All (7) 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)
2:C:501:SO4:O2	2:C:501:SO4:O4[2_556]	0.39	1.81
2:C:501:SO4:O1	2:C:501:SO4:O3[2_556]	0.65	1.55
2:C:501:SO4:S	2:C:501:SO4:O3[2_556]	1.58	0.62
2:C:501:SO4:S	2:C:501:SO4:O1[2_556]	1.59	0.61
2:C:501:SO4:S	2:C:501:SO4:O4[2_556]	1.60	0.60
2:C:501:SO4:S	2:C:501:SO4:O2[2_556]	1.60	0.60
2:C:501:SO4:O3	2:C:501:SO4:O3[2_556]	2.06	0.14

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	358/407 (88%)	337 (94%)	18 (5%)	3 (1%)	16	44
1	B	364/407 (89%)	344 (94%)	15 (4%)	5 (1%)	9	30
1	C	361/407 (89%)	336 (93%)	23 (6%)	2 (1%)	21	51
1	D	351/407 (86%)	331 (94%)	18 (5%)	2 (1%)	21	51
All	All	1434/1628 (88%)	1348 (94%)	74 (5%)	12 (1%)	16	44

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	THR
1	C	211	LYS
1	A	17	ALA
1	A	95	ASP
1	C	17	ALA
1	D	281	ASP
1	B	404	ALA
1	D	256	SER
1	B	10	SER
1	B	391	GLU
1	B	204	ASN
1	B	253	GLY

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	288/316 (91%)	288 (100%)	0	100	100
1	B	291/316 (92%)	288 (99%)	3 (1%)	68	89
1	C	290/316 (92%)	285 (98%)	5 (2%)	53	82
1	D	283/316 (90%)	282 (100%)	1 (0%)	84	94
All	All	1152/1264 (91%)	1143 (99%)	9 (1%)	73	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	254	TYR
1	B	308	GLU
1	B	391	GLU
1	C	83	ARG
1	C	254	TYR
1	C	255	ASN
1	C	282	LEU
1	C	308	GLU
1	D	281	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	89	GLN
1	A	205	GLN
1	A	320	HIS
1	B	167	HIS
1	C	252	HIS
1	C	320	HIS
1	C	377	HIS
1	D	240	HIS
1	D	386	GLN

5.3.3 RNA ⓘ

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	SO4	B	501	-	4,4,4	0.22	0	6,6,6	0.42	0
2	SO4	D	501	-	4,4,4	0.28	0	6,6,6	0.34	0
2	SO4	C	502	-	4,4,4	1.36	0	6,6,6	0.41	0
2	SO4	B	502	-	4,4,4	1.54	1 (25%)	6,6,6	0.76	0
2	SO4	C	501	-	4,4,4	2.07	2 (50%)	6,6,6	0.77	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	SO4	O2-S	2.61	1.60	1.44
2	C	501	SO4	O1-S	2.54	1.59	1.44
2	B	502	SO4	O1-S	2.05	1.57	1.44

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	SO4	1	0
2	C	501	SO4	0	7

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	366/407 (89%)	0.53	16 (4%)	39	30	22, 48, 85, 116	0
1	B	370/407 (90%)	0.52	26 (7%)	22	18	24, 44, 96, 151	0
1	C	369/407 (90%)	0.75	31 (8%)	17	14	29, 53, 112, 150	0
1	D	361/407 (88%)	0.66	34 (9%)	14	12	25, 53, 99, 160	0
All	All	1466/1628 (90%)	0.62	107 (7%)	21	17	22, 50, 99, 160	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	374	LEU	5.3
1	C	12	THR	5.0
1	B	252	HIS	4.9
1	B	406	LEU	4.6
1	B	393	TYR	4.6
1	A	285	VAL	4.1
1	B	285	VAL	4.0
1	C	285	VAL	4.0
1	B	255	ASN	4.0
1	B	15	SER	4.0
1	C	406	LEU	4.0
1	D	294	TRP	3.9
1	D	285	VAL	3.7
1	A	315	ARG	3.6
1	D	283	PRO	3.6
1	C	10	SER	3.5
1	B	2	THR	3.5
1	C	252	HIS	3.5
1	B	11	LEU	3.4
1	D	280	ALA	3.4
1	D	11	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	282	LEU	3.4
1	C	15	SER	3.3
1	C	255	ASN	3.3
1	B	254	TYR	3.2
1	C	254	TYR	3.2
1	D	347	SER	3.2
1	B	391	GLU	3.2
1	C	11	LEU	3.1
1	A	226	PRO	3.1
1	D	5	TYR	3.1
1	B	253	GLY	3.1
1	A	279	ILE	3.1
1	D	279	ILE	3.0
1	A	282	LEU	2.9
1	B	284	GLU	2.9
1	A	11	LEU	2.9
1	C	210	ALA	2.8
1	C	34	GLY	2.8
1	B	405	ARG	2.8
1	A	98	LEU	2.7
1	C	393	TYR	2.7
1	D	48	ARG	2.6
1	A	244	THR	2.6
1	C	276	PRO	2.6
1	C	282	LEU	2.6
1	D	286	ASN	2.6
1	D	217	ARG	2.6
1	D	281	ASP	2.6
1	D	247	VAL	2.5
1	C	267	LEU	2.5
1	C	287	ARG	2.5
1	C	217	ARG	2.5
1	D	288	ASP	2.5
1	B	347	SER	2.5
1	D	295	ARG	2.4
1	D	17	ALA	2.4
1	D	16	ASP	2.4
1	C	13	SER	2.4
1	A	284	GLU	2.4
1	B	377	HIS	2.4
1	C	333	ASP	2.4
1	A	335	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	346	GLU	2.3
1	D	7	LYS	2.3
1	D	8	LYS	2.3
1	C	16	ASP	2.3
1	B	250	ALA	2.3
1	B	346	GLU	2.3
1	D	404	ALA	2.3
1	A	84	ARG	2.3
1	B	283	PRO	2.3
1	C	46	PHE	2.3
1	D	89	GLN	2.3
1	B	13	SER	2.3
1	B	251	GLU	2.2
1	D	96	VAL	2.2
1	D	276	PRO	2.2
1	D	275	ILE	2.2
1	B	100	VAL	2.2
1	C	18	SER	2.2
1	D	10	SER	2.2
1	C	14	LYS	2.2
1	C	288	ASP	2.2
1	A	347	SER	2.2
1	C	189	GLY	2.2
1	D	374	LEU	2.2
1	D	19	ASP	2.2
1	D	258	VAL	2.2
1	D	235	ARG	2.1
1	C	286	ASN	2.1
1	B	14	LYS	2.1
1	B	282	LEU	2.1
1	D	154	PRO	2.1
1	C	243	THR	2.1
1	C	311	ALA	2.1
1	D	250	ALA	2.1
1	D	297	TYR	2.1
1	A	15	SER	2.1
1	A	242	VAL	2.1
1	B	89	GLN	2.1
1	D	255	ASN	2.1
1	C	271	VAL	2.0
1	B	404	ALA	2.0
1	A	304	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	345	GLU	2.0
1	A	278	TYR	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	SO4	D	501	5/5	0.67	0.23	99,101,102,103	0
2	SO4	C	501	5/5	0.79	0.18	87,88,98,124	1
2	SO4	C	502	5/5	0.80	0.31	80,88,90,112	0
2	SO4	B	502	5/5	0.80	0.24	67,72,77,108	0
2	SO4	B	501	5/5	0.84	0.10	60,64,86,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.