



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:28 AM UTC

PDB ID : 3TCS / pdb_00003tcs
Title : Crystal structure of a putative racemase from *Roseobacter denitrificans*
Authors : Eswaramoorthy, S.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; LaFleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYS-GRC)
Deposited on : 2011-08-09
Resolution : 1.88 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

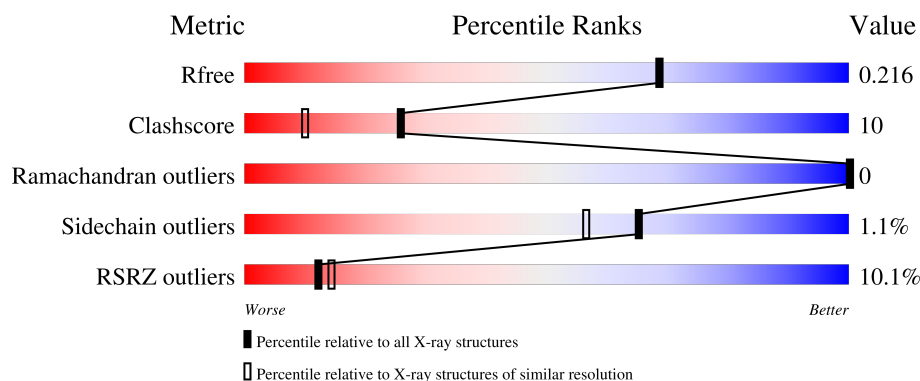
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	388	16% 71% 22% 6%
1	B	388	3% 78% 15% 5%

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
4	DAL	A	370	-	-	X	-
4	DAL	B	370	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6089 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 Racemase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2900	1825	508	550	17			
1	B	367	Total	C	N	O	S	0	0	0
			2906	1828	509	552	17			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP Q161M1
A	-20	HIS	-	expression tag	UNP Q161M1
A	-19	HIS	-	expression tag	UNP Q161M1
A	-18	HIS	-	expression tag	UNP Q161M1
A	-17	HIS	-	expression tag	UNP Q161M1
A	-16	HIS	-	expression tag	UNP Q161M1
A	-15	HIS	-	expression tag	UNP Q161M1
A	-14	SER	-	expression tag	UNP Q161M1
A	-13	SER	-	expression tag	UNP Q161M1
A	-12	GLY	-	expression tag	UNP Q161M1
A	-11	VAL	-	expression tag	UNP Q161M1
A	-10	ASP	-	expression tag	UNP Q161M1
A	-9	LEU	-	expression tag	UNP Q161M1
A	-8	GLY	-	expression tag	UNP Q161M1
A	-7	THR	-	expression tag	UNP Q161M1
A	-6	GLU	-	expression tag	UNP Q161M1
A	-5	ASN	-	expression tag	UNP Q161M1
A	-4	LEU	-	expression tag	UNP Q161M1
A	-3	TYR	-	expression tag	UNP Q161M1
A	-2	PHE	-	expression tag	UNP Q161M1
A	-1	GLN	-	expression tag	UNP Q161M1
A	0	SER	-	expression tag	UNP Q161M1
B	-21	MET	-	expression tag	UNP Q161M1
B	-20	HIS	-	expression tag	UNP Q161M1
B	-19	HIS	-	expression tag	UNP Q161M1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	HIS	-	expression tag	UNP Q161M1
B	-17	HIS	-	expression tag	UNP Q161M1
B	-16	HIS	-	expression tag	UNP Q161M1
B	-15	HIS	-	expression tag	UNP Q161M1
B	-14	SER	-	expression tag	UNP Q161M1
B	-13	SER	-	expression tag	UNP Q161M1
B	-12	GLY	-	expression tag	UNP Q161M1
B	-11	VAL	-	expression tag	UNP Q161M1
B	-10	ASP	-	expression tag	UNP Q161M1
B	-9	LEU	-	expression tag	UNP Q161M1
B	-8	GLY	-	expression tag	UNP Q161M1
B	-7	THR	-	expression tag	UNP Q161M1
B	-6	GLU	-	expression tag	UNP Q161M1
B	-5	ASN	-	expression tag	UNP Q161M1
B	-4	LEU	-	expression tag	UNP Q161M1
B	-3	TYR	-	expression tag	UNP Q161M1
B	-2	PHE	-	expression tag	UNP Q161M1
B	-1	GLN	-	expression tag	UNP Q161M1
B	0	SER	-	expression tag	UNP Q161M1

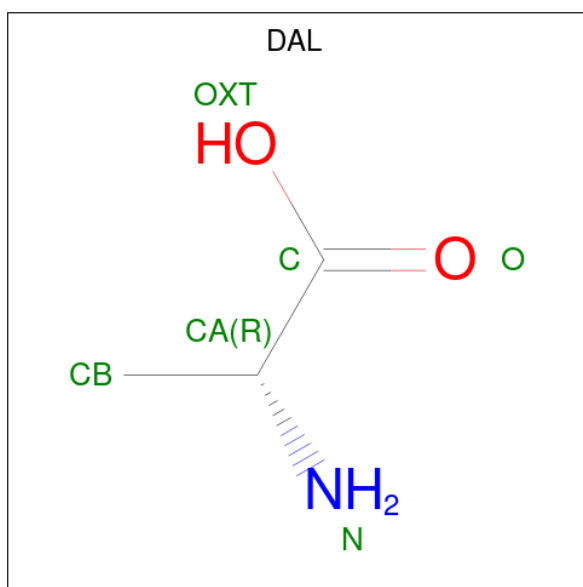
- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	B	2	Total Mg 2 2	0	0

- Molecule 4 is D-ALANINE (CCD ID: DAL) (formula: C₃H₇NO₂).



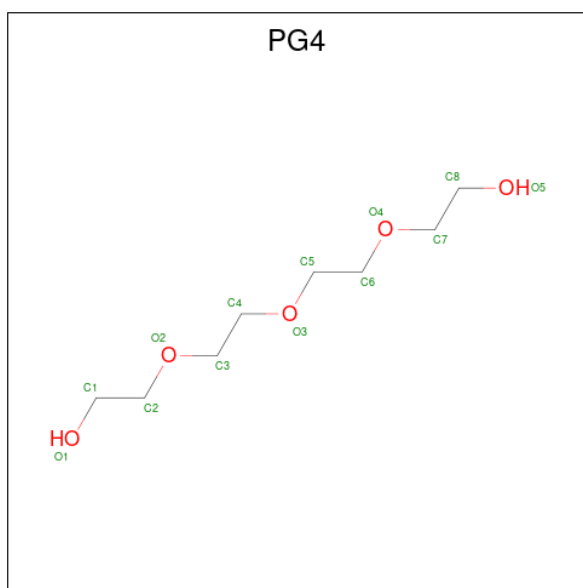
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			5	3	1	1		
4	B	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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



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

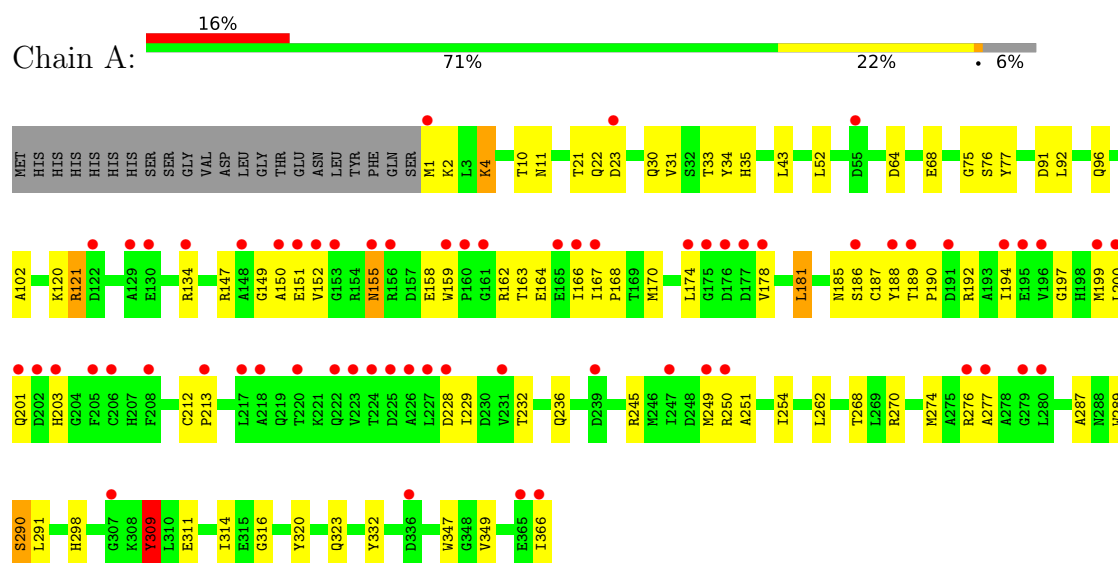
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	84	Total	O	0	0
			84	84		
7	B	145	Total	O	0	0
			145	145		

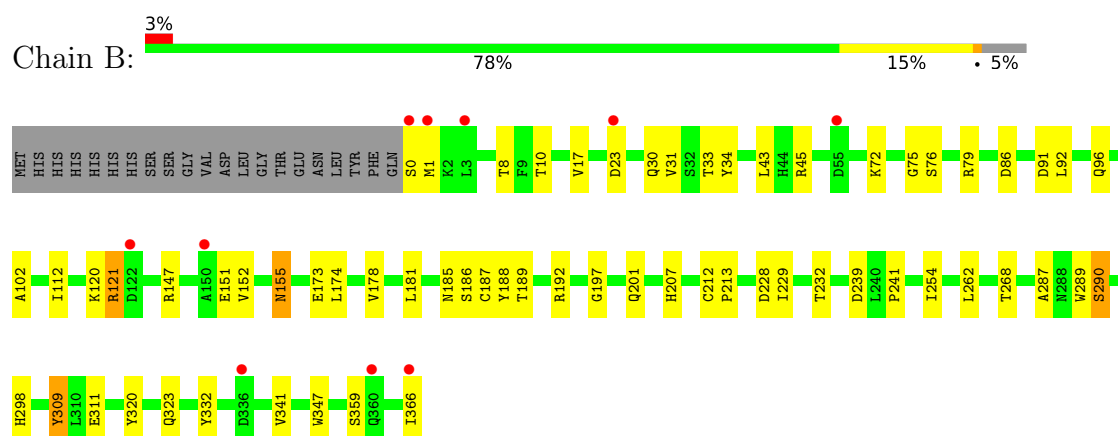
3 Residue-property plots [i](#)

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: Racemase, putative



• Molecule 1: Racemase, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	182.49Å 64.75Å 76.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.45 – 1.88 43.45 – 1.88	Depositor EDS
% Data completeness (in resolution range)	97.2 (43.45-1.88) 97.2 (43.45-1.88)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 1.87Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.195 , 0.216 0.196 , 0.216	Depositor DCC
R_{free} test set	3703 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.5	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	0.94	EDS
Total number of atoms	6089	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: DAL, MG, CL, PG4, GOL

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	0.34	0/2969	0.94	16/4037 (0.4%)
1	B	0.36	0/2975	0.94	12/4045 (0.3%)
All	All	0.35	0/5944	0.94	28/8082 (0.3%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	SER	N-CA-C	9.04	120.74	111.07
1	A	76	SER	N-CA-C	9.02	120.80	110.97
1	B	188	TYR	N-CA-C	8.92	123.72	110.52
1	B	290	SER	N-CA-C	-8.44	96.62	109.79
1	B	189	THR	N-CA-C	-8.13	99.46	110.36
1	A	290	SER	N-CA-C	-8.08	97.19	109.79
1	A	332	TYR	N-CA-C	7.56	121.11	112.57
1	A	188	TYR	N-CA-C	6.68	120.77	110.42
1	B	121	ARG	N-CA-C	-6.37	106.10	114.31
1	B	120	LYS	N-CA-C	6.32	119.83	110.48
1	B	187	CYS	N-CA-C	6.29	119.42	111.69
1	A	287	ALA	N-CA-C	6.25	120.94	112.88
1	B	287	ALA	N-CA-C	6.22	120.90	112.88
1	A	189	THR	N-CA-C	-6.16	102.10	110.36
1	A	11	ASN	N-CA-C	-5.98	100.51	108.34
1	A	309	TYR	N-CA-C	5.78	116.92	108.14
1	A	120	LYS	N-CA-C	5.60	118.77	110.48
1	B	332	TYR	N-CA-C	5.56	119.60	112.26
1	B	10	THR	N-CA-C	5.54	117.61	109.24
1	A	166	ILE	N-CA-C	5.53	116.26	110.62
1	A	10	THR	N-CA-C	5.51	117.17	108.96
1	A	75	GLY	N-CA-C	5.39	117.83	111.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	GLU	N-CA-C	5.37	117.22	111.36
1	B	359	SER	N-CA-C	5.31	117.38	110.53
1	A	316	GLY	CA-C-N	5.26	124.93	119.56
1	A	316	GLY	C-N-CA	5.26	124.93	119.56
1	A	121	ARG	N-CA-C	-5.23	107.92	114.56
1	A	77	TYR	N-CA-C	5.12	117.25	111.11

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	2900	0	2818	70	0
1	B	2906	0	2823	43	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	5	0	6	4	0
4	B	5	0	6	4	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	A	13	0	18	0	0
6	B	13	0	18	0	0
7	A	84	0	0	0	0
7	B	145	0	0	0	0
All	All	6089	0	5705	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 10.

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:B:121:ARG:HH22	1:B:185:ASN:HD22	1.06	0.93
1:A:1:MET:HE1	1:A:23:ASP:H	1.31	0.92
1:A:1:MET:HE2	1:A:21:THR:HB	1.58	0.86
1:B:311:GLU:OE2	4:B:370:DAL:HB2	1.80	0.81
1:B:201:GLN:HE22	1:B:228:ASP:H	1.30	0.80
1:A:121:ARG:HH22	1:A:185:ASN:ND2	1.81	0.79
1:B:147:ARG:HH11	1:B:185:ASN:HD21	1.29	0.79
1:A:201:GLN:HE22	1:A:228:ASP:H	1.34	0.75
1:A:102:ALA:H	1:A:298:HIS:HD2	1.35	0.73
1:B:0:SER:O	1:B:1:MET:HE2	1.89	0.73
1:B:102:ALA:H	1:B:298:HIS:HD2	1.37	0.72
1:A:232:THR:HG22	1:A:254:ILE:HB	1.71	0.72
1:A:1:MET:HE1	1:A:23:ASP:N	2.04	0.71
1:A:163:THR:O	1:A:167:ILE:HG12	1.90	0.71
1:A:311:GLU:OE2	4:A:370:DAL:HB2	1.92	0.70
1:A:147:ARG:HH11	1:A:185:ASN:HD21	1.41	0.69
1:B:121:ARG:NH2	1:B:185:ASN:HD22	1.88	0.68
1:A:190:PRO:O	1:A:194:ILE:HG13	1.95	0.67
1:A:1:MET:HG2	1:A:2:LYS:H	1.60	0.67
1:B:201:GLN:NE2	1:B:228:ASP:H	1.93	0.66
1:B:239:ASP:OD2	1:B:241:PRO:HG2	1.95	0.66
1:A:250:ARG:HH11	1:A:250:ARG:HG3	1.60	0.65
1:A:1:MET:HE3	1:A:22:GLN:HB2	1.78	0.64
1:B:201:GLN:HE21	1:B:229:ILE:H	1.46	0.63
1:A:121:ARG:HH12	1:A:185:ASN:HD22	1.46	0.62
1:A:197:GLY:O	1:A:201:GLN:HG3	1.99	0.62
1:A:64:ASP:O	1:A:68:GLU:HG3	2.01	0.61
1:A:236:GLN:HE21	1:B:72:LYS:HD3	1.65	0.61
1:A:201:GLN:HE21	1:A:229:ILE:H	1.48	0.60
1:B:0:SER:HB3	1:B:23:ASP:OD1	2.02	0.60
1:A:309:TYR:CD2	1:A:309:TYR:N	2.71	0.58
1:A:201:GLN:NE2	1:A:228:ASP:H	2.00	0.58
1:A:366:ILE:HG13	1:A:366:ILE:OXT	2.06	0.56
1:B:92:LEU:O	1:B:96:GLN:HG3	2.07	0.54
1:A:121:ARG:O	1:A:158:GLU:HG2	2.06	0.54
1:B:147:ARG:HH12	4:B:370:DAL:HA	1.73	0.54
1:A:134:ARG:HH11	1:A:134:ARG:HG3	1.74	0.53
1:B:186:SER:HB3	1:B:213:PRO:HA	1.91	0.53
1:B:147:ARG:HH22	4:B:370:DAL:HA	1.74	0.52
1:A:167:ILE:HB	1:A:168:PRO:CD	2.39	0.52
1:A:245:ARG:O	1:A:249:MET:HG2	2.09	0.52
1:A:1:MET:HG2	1:A:2:LYS:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ILE:HB	1:A:168:PRO:HD3	1.90	0.52
1:A:186:SER:HB3	1:A:213:PRO:HA	1.92	0.52
1:A:250:ARG:HG3	1:A:250:ARG:NH1	2.24	0.52
1:A:91:ASP:HB2	1:A:347:TRP:CD1	2.45	0.51
1:A:167:ILE:HD12	1:A:200:LEU:HD23	1.93	0.50
1:A:164:GLU:HG3	1:A:199:MET:HE1	1.93	0.50
1:A:121:ARG:HD3	1:A:149:GLY:O	2.12	0.50
1:B:30:GLN:HG2	1:B:31:VAL:O	2.13	0.49
1:A:262:LEU:HD23	1:A:268:THR:HA	1.95	0.48
1:A:167:ILE:HD12	1:A:200:LEU:CD2	2.44	0.48
1:B:147:ARG:HH22	4:B:370:DAL:CB	2.26	0.48
1:B:309:TYR:N	1:B:309:TYR:CD2	2.80	0.48
1:A:249:MET:HE2	1:A:251:ALA:HB2	1.94	0.48
1:A:92:LEU:O	1:A:96:GLN:HG3	2.13	0.48
1:B:91:ASP:HB2	1:B:347:TRP:CD1	2.49	0.48
1:A:181:LEU:HD12	1:A:181:LEU:N	2.29	0.47
1:A:170:MET:HE3	1:A:174:LEU:HD22	1.96	0.47
1:A:4:LYS:NZ	1:A:21:THR:O	2.48	0.47
1:A:155:ASN:HD21	1:A:192:ARG:HB3	1.80	0.47
1:B:181:LEU:HD12	1:B:181:LEU:N	2.30	0.47
1:A:147:ARG:HH22	4:A:370:DAL:CB	2.28	0.47
1:B:43:LEU:HD23	1:B:43:LEU:C	2.40	0.46
1:B:366:ILE:C	1:B:366:ILE:HD12	2.40	0.46
1:A:320:TYR:O	1:A:323:GLN:HG2	2.16	0.46
1:B:121:ARG:HH22	1:B:185:ASN:ND2	1.90	0.46
1:B:181:LEU:HG	1:B:207:HIS:HB3	1.97	0.46
1:B:75:GLY:O	1:B:79:ARG:HD3	2.16	0.46
1:A:43:LEU:C	1:A:43:LEU:HD23	2.40	0.46
1:A:33:THR:O	1:A:34:TYR:HB2	2.16	0.45
1:A:35:HIS:CD2	1:B:45:ARG:HH11	2.35	0.45
1:A:1:MET:CE	1:A:23:ASP:H	2.16	0.45
1:A:168:PRO:HB3	1:A:203:HIS:NE2	2.32	0.45
1:A:147:ARG:HH12	4:A:370:DAL:C	2.30	0.45
1:A:232:THR:CG2	1:A:254:ILE:HB	2.44	0.45
1:B:33:THR:O	1:B:34:TYR:HB2	2.18	0.44
1:A:174:LEU:HB3	1:A:178:VAL:HG21	2.00	0.44
1:A:155:ASN:HD22	1:A:155:ASN:HA	1.54	0.44
1:A:35:HIS:HD2	1:B:45:ARG:HH11	1.65	0.43
1:A:150:ALA:O	1:A:187:CYS:HB2	2.18	0.43
1:B:0:SER:HB2	1:B:23:ASP:HB3	2.01	0.43
1:B:212:CYS:O	1:B:213:PRO:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:GLY:O	1:B:201:GLN:HG3	2.19	0.42
1:A:212:CYS:HB3	1:A:213:PRO:HD2	2.00	0.42
1:A:30:GLN:HG2	1:A:31:VAL:O	2.19	0.42
1:A:151:GLU:O	1:A:152:VAL:C	2.62	0.42
1:A:134:ARG:HG3	1:A:134:ARG:NH1	2.34	0.42
1:A:147:ARG:HH12	4:A:370:DAL:HA	1.83	0.42
1:B:174:LEU:HB3	1:B:178:VAL:HG21	2.01	0.42
1:B:151:GLU:O	1:B:152:VAL:C	2.62	0.41
1:B:232:THR:HG22	1:B:254:ILE:HB	2.01	0.41
1:A:159:TRP:NE1	1:A:162:ARG:HB2	2.35	0.41
1:A:276:ARG:HG3	1:A:277:ALA:N	2.35	0.41
1:B:8:THR:HG22	1:B:17:VAL:HG22	2.02	0.41
1:B:112:ILE:HD11	1:B:341:VAL:HG23	2.02	0.41
1:A:152:VAL:O	1:A:152:VAL:HG12	2.20	0.41
1:A:159:TRP:CD1	1:A:162:ARG:HB2	2.56	0.41
1:A:289:TRP:C	1:A:290:SER:O	2.60	0.41
1:A:291:LEU:HD21	1:A:349:VAL:HG11	2.03	0.41
1:A:314:ILE:C	1:A:314:ILE:HD12	2.45	0.41
1:B:155:ASN:HD22	1:B:155:ASN:HA	1.57	0.41
1:B:155:ASN:HD21	1:B:192:ARG:HB3	1.86	0.41
1:B:201:GLN:NE2	1:B:229:ILE:H	2.16	0.41
1:B:289:TRP:C	1:B:290:SER:O	2.61	0.40
1:A:52:LEU:HB3	1:A:366:ILE:CG2	2.51	0.40
1:A:212:CYS:HB3	1:A:213:PRO:CD	2.51	0.40
1:A:270:ARG:O	1:A:274:MET:HG3	2.21	0.40
1:B:262:LEU:HD23	1:B:268:THR:HA	2.03	0.40
1:B:320:TYR:O	1:B:323:GLN:HG2	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	364/388 (94%)	353 (97%)	11 (3%)	0	100	100
1	B	365/388 (94%)	353 (97%)	12 (3%)	0	100	100
All	All	729/776 (94%)	706 (97%)	23 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	307/327 (94%)	303 (99%)	4 (1%)	61	50
1	B	308/327 (94%)	305 (99%)	3 (1%)	68	60
All	All	615/654 (94%)	608 (99%)	7 (1%)	65	56

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

Mol	Chain	Res	Type
1	A	4	LYS
1	A	155	ASN
1	A	181	LEU
1	A	309	TYR
1	B	86	ASP
1	B	155	ASN
1	B	309	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	46	GLN
1	A	139	GLN
1	A	155	ASN
1	A	185	ASN
1	A	201	GLN

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Mol	Chain	Res	Type
1	A	236	GLN
1	A	298	HIS
1	A	360	GLN
1	B	22	GLN
1	B	155	ASN
1	B	185	ASN
1	B	201	GLN
1	B	298	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	DAL	A	370	3	3,4,5	0.21	0	2,4,6	0.80	0
5	GOL	A	371	-	5,5,5	0.54	0	5,5,5	0.26	0
4	DAL	B	370	3	3,4,5	0.15	0	2,4,6	0.91	0
6	PG4	B	372	-	12,12,12	0.61	0	11,11,11	0.99	0
5	GOL	B	371	-	5,5,5	0.43	0	5,5,5	0.19	0
6	PG4	A	372	-	12,12,12	0.63	0	11,11,11	1.01	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
4	DAL	A	370	3	-	0/1/2/4	-
5	GOL	A	371	-	-	0/4/4/4	-
4	DAL	B	370	3	-	0/1/2/4	-
6	PG4	B	372	-	-	1/10/10/10	-
5	GOL	B	371	-	-	0/4/4/4	-
6	PG4	A	372	-	-	1/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	372	PG4	O4-C7-C8-O5
6	A	372	PG4	O4-C7-C8-O5

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	370	DAL	4	0
4	B	370	DAL	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	366/388 (94%)	0.69	64 (17%) 4 4	9, 20, 35, 40	0
1	B	367/388 (94%)	-0.19	10 (2%) 56 61	6, 12, 23, 37	0
All	All	733/776 (94%)	0.25	74 (10%) 12 14	6, 15, 33, 40	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	366	ILE	5.0
1	B	366	ILE	4.9
1	A	199	MET	4.3
1	B	0	SER	4.1
1	A	150	ALA	4.0
1	B	122	ASP	3.9
1	A	176	ASP	3.8
1	A	156	ARG	3.8
1	A	226	ALA	3.7
1	A	122	ASP	3.7
1	A	152	VAL	3.5
1	A	277	ALA	3.3
1	A	280	LEU	3.2
1	A	203	HIS	3.2
1	B	1	MET	3.1
1	A	276	ARG	3.1
1	A	153	GLY	3.0
1	A	160	PRO	3.0
1	A	228	ASP	3.0
1	A	1	MET	2.9
1	A	202	ASP	2.9
1	A	159	TRP	2.9
1	A	217	LEU	2.9
1	A	196	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	194	ILE	2.7
1	A	177	ASP	2.7
1	A	167	ILE	2.7
1	A	148	ALA	2.6
1	A	191	ASP	2.6
1	A	200	LEU	2.6
1	A	218	ALA	2.6
1	A	166	ILE	2.6
1	A	247	ILE	2.6
1	A	206	CYS	2.5
1	A	208	PHE	2.5
1	A	336	ASP	2.5
1	B	336	ASP	2.5
1	A	195	GLU	2.5
1	B	23	ASP	2.5
1	A	129	ALA	2.4
1	A	165	GLU	2.4
1	A	231	VAL	2.4
1	A	222	GLN	2.4
1	A	178	VAL	2.4
1	A	239	ASP	2.3
1	A	174	LEU	2.3
1	A	279	GLY	2.3
1	B	55	ASP	2.3
1	A	55	ASP	2.3
1	A	224	THR	2.3
1	A	223	VAL	2.2
1	A	205	PHE	2.2
1	A	250	ARG	2.2
1	A	220	THR	2.2
1	B	3	LEU	2.2
1	A	155	ASN	2.2
1	A	249	MET	2.2
1	A	365	GLU	2.1
1	B	150	ALA	2.1
1	A	188	TYR	2.1
1	A	189	THR	2.1
1	A	161	GLY	2.1
1	A	175	GLY	2.1
1	A	130	GLU	2.1
1	A	227	LEU	2.1
1	A	23	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	186	SER	2.1
1	A	201	GLN	2.1
1	A	213	PRO	2.1
1	A	225	ASP	2.1
1	A	134	ARG	2.1
1	A	151	GLU	2.0
1	A	307	GLY	2.0
1	B	360	GLN	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
6	PG4	A	372	13/13	0.82	0.14	25,27,32,32	0
4	DAL	B	370	5/6	0.85	0.14	9,11,13,20	0
4	DAL	A	370	5/6	0.85	0.14	17,17,20,24	0
6	PG4	B	372	13/13	0.89	0.11	20,23,30,32	0
5	GOL	A	371	6/6	0.90	0.11	23,25,26,27	0
5	GOL	B	371	6/6	0.90	0.11	21,23,24,26	0
3	MG	A	369	1/1	0.93	0.06	35,35,35,35	0
3	MG	B	369	1/1	0.96	0.04	14,14,14,14	0
2	CL	B	367	1/1	0.97	0.06	22,22,22,22	0
3	MG	A	368	1/1	0.97	0.03	18,18,18,18	0
3	MG	B	368	1/1	0.98	0.03	10,10,10,10	0
2	CL	A	367	1/1	0.99	0.03	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.