



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:31 AM UTC

PDB ID : 2XDQ / pdb_00002xdq
Title : Dark Operative Protochlorophyllide Oxidoreductase (ChlN-ChlB)2 Complex
Authors : Broecker, M.J.; Schomburg, S.; Heinz, D.W.; Jahn, D.; Schubert, W.-D.; Moser, J.
Deposited on : 2010-05-06
Resolution : 2.40 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

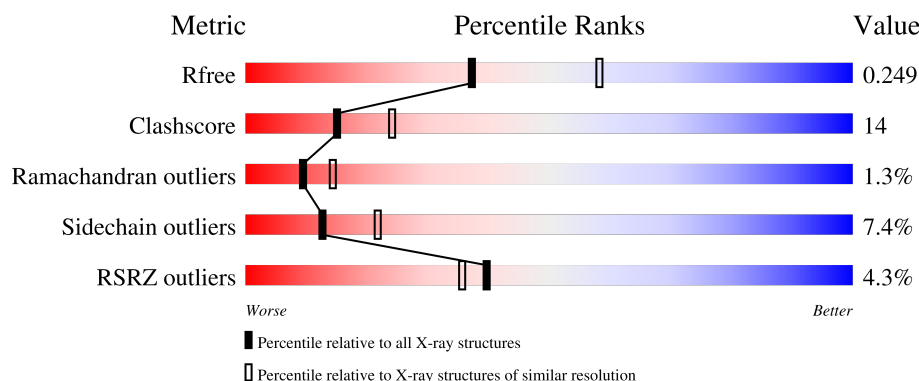
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	460	5% 62% 26% • 8%
2	B	511	3% 58% 24% • 14%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7097 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 LIGHT-INDEPENDENT PROTOCHLOROPHYLLIDE REDUCTASE SUBUNIT N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	9	0
			3401	2186	579	613	23			

- Molecule 2 is a protein called LIGHT-INDEPENDENT PROTOCHLOROPHYLLIDE REDUCTASE SUBUNIT B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	440	Total	C	N	O	S	0	12	0
			3533	2237	635	640	21			

There are 3 discrepancies between the modelled and reference sequences:

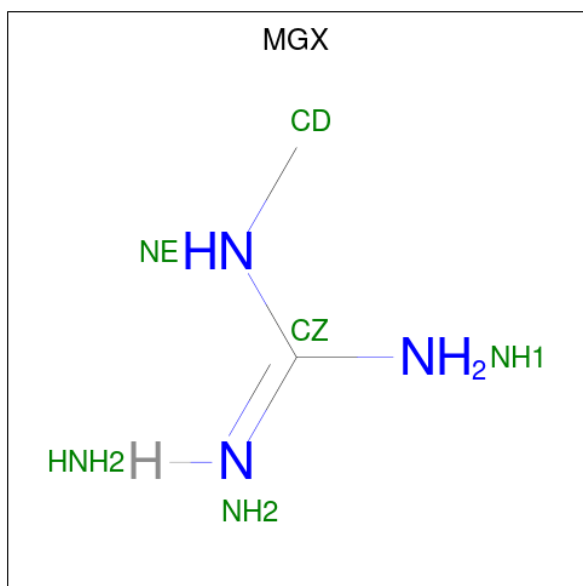
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	ALA	-	expression tag	UNP Q8DGC6
B	-1	ALA	-	expression tag	UNP Q8DGC6
B	0	ALA	-	expression tag	UNP Q8DGC6

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is 1-METHYLGUANIDINE (CCD ID: MGX) (formula: $C_2H_7N_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	2	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

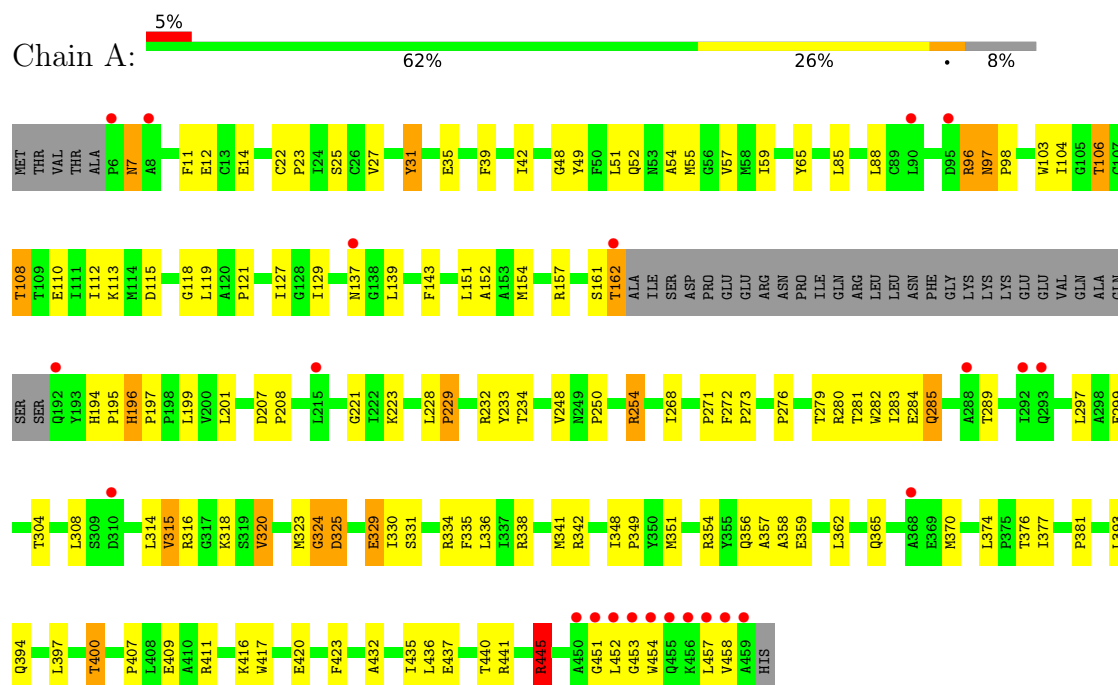
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	37	Total	O	0	0
			37	37		
6	B	103	Total	O	0	0
			103	103		

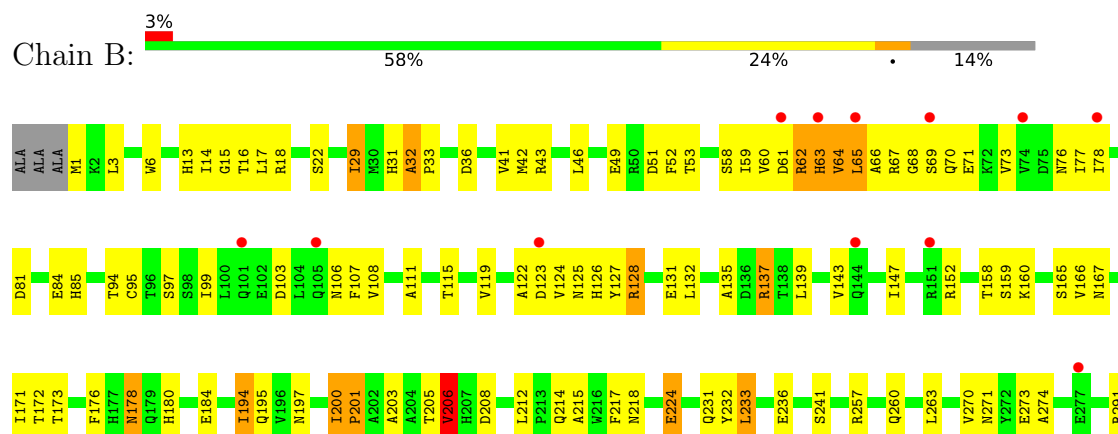
3 Residue-property plots [i](#)

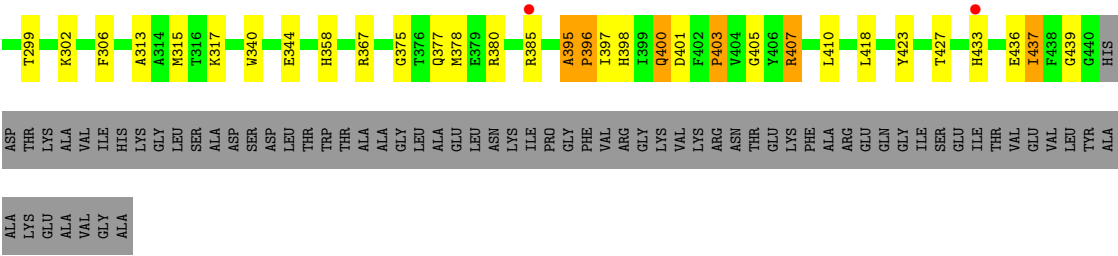
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: LIGHT-INDEPENDENT PROTOCHLOROPHYLLIDE REDUCTASE SUBUNIT N



• Molecule 2: LIGHT-INDEPENDENT PROTOCHLOROPHYLLIDE REDUCTASE SUBUNIT B





4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	192.09Å 192.09Å 132.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	103.65 – 2.40 103.65 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.6 (103.65-2.40) 98.6 (103.65-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.201 , 0.257 0.198 , 0.249	Depositor DCC
R_{free} test set	2817 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.523	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 69.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7097	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: SO4, MGX, SF4

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	1.15	8/3504 (0.2%)	1.24	15/4755 (0.3%)
2	B	1.15	9/3642 (0.2%)	1.21	12/4938 (0.2%)
All	All	1.15	17/7146 (0.2%)	1.23	27/9693 (0.3%)

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
2	B	0	4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	203	ALA	CA-CB	9.26	1.67	1.53
2	B	212	LEU	N-CA	7.15	1.53	1.46
1	A	27	VAL	CA-CB	5.96	1.61	1.54
1	A	103	TRP	CA-C	-5.78	1.45	1.52
2	B	85	HIS	C-O	-5.71	1.21	1.23
2	B	274	ALA	CA-CB	5.67	1.62	1.53
2	B	139	LEU	CA-C	5.56	1.60	1.52
1	A	435	ILE	CA-CB	5.55	1.60	1.54
2	B	32	ALA	CA-CB	5.39	1.62	1.54
1	A	25	SER	N-CA	5.33	1.53	1.46
2	B	135	ALA	CA-CB	5.26	1.62	1.53
1	A	54	ALA	C-O	-5.24	1.18	1.24
1	A	325	ASP	N-CA	5.22	1.52	1.46
1	A	97	ASN	C-O	5.18	1.26	1.23
2	B	41	VAL	CA-CB	-5.17	1.48	1.54
2	B	403	PRO	CB-CG	5.08	1.75	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	GLY	N-CA	-5.02	1.39	1.45

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	LEU	CA-C-N	21.80	179.32	127.00
1	A	228	LEU	C-N-CA	21.80	179.32	127.00
1	A	228	LEU	C-N-CD	-20.43	75.66	120.60
2	B	395	ALA	CA-C-N	19.88	144.68	119.84
2	B	395	ALA	C-N-CA	19.88	144.68	119.84
2	B	200	ILE	CA-C-N	12.69	135.70	119.84
2	B	200	ILE	C-N-CA	12.69	135.70	119.84
2	B	395	ALA	C-N-CD	-11.18	79.15	125.00
2	B	200	ILE	C-N-CD	-9.15	87.50	125.00
1	A	323	MET	CA-C-N	-8.77	112.01	120.34
1	A	323	MET	C-N-CA	-8.77	112.01	120.34
2	B	270	VAL	N-CA-C	7.46	118.55	108.11
2	B	178	ASN	N-CA-C	7.21	118.78	111.07
1	A	129	ILE	N-CA-C	7.04	115.56	107.89
1	A	323	MET	N-CA-C	-7.00	98.63	109.76
2	B	396	PRO	CA-N-CD	-6.82	102.45	112.00
1	A	400	THR	N-CA-C	6.43	117.91	108.14
2	B	85	HIS	CB-CA-C	-5.99	105.79	111.00
1	A	35	GLU	N-CA-C	5.76	118.33	111.71
1	A	324	GLY	N-CA-C	5.46	119.19	112.14
1	A	97	ASN	CA-C-N	5.44	125.42	120.03
1	A	97	ASN	C-N-CA	5.44	125.42	120.03
1	A	457	LEU	N-CA-C	5.39	117.79	110.88
2	B	194	ILE	CB-CA-C	-5.28	103.91	111.31
1	A	445	ARG	CB-CG-CD	-5.16	99.44	111.30
1	A	437	GLU	N-CA-C	-5.07	105.19	111.33
2	B	405	GLY	N-CA-C	-5.01	106.17	111.93

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	200	ILE	Mainchain,Peptide
2	B	395	ALA	Mainchain,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	3401	0	3456	91	0
2	B	3533	0	3553	107	0
3	A	8	0	0	0	0
4	A	5	0	6	0	0
5	B	10	0	0	0	0
6	A	37	0	0	0	0
6	B	103	0	0	5	0
All	All	7097	0	7015	192	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 14.

All (192) 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)
2:B:403:PRO:CB	2:B:403:PRO:CG	1.75	1.39
2:B:128[A]:ARG:HH11	2:B:128[A]:ARG:HG3	1.09	1.15
2:B:64:VAL:HG13	2:B:69:SER:OG	1.51	1.10
2:B:64:VAL:HA	2:B:68:GLY:HA3	1.37	1.06
2:B:128[A]:ARG:HH11	2:B:128[A]:ARG:CG	1.67	1.06
1:A:157[B]:ARG:HG3	1:A:157[B]:ARG:NH1	1.64	1.05
1:A:157[B]:ARG:HH11	1:A:157[B]:ARG:CG	1.66	1.05
1:A:49:TYR:CE2	2:B:42[A]:MET:HE1	1.91	1.04
1:A:96[A]:ARG:HH11	1:A:96[A]:ARG:CG	1.71	1.03
2:B:70:GLN:HB2	2:B:107:PHE:CZ	1.94	1.02
1:A:271:PRO:HG2	1:A:281:THR:HG21	1.43	1.00
1:A:157[B]:ARG:HG3	1:A:157[B]:ARG:HH11	0.85	1.00
1:A:96[A]:ARG:HH11	1:A:96[A]:ARG:HG3	1.27	0.98
1:A:137:ASN:OD1	1:A:139:LEU:HB2	1.64	0.98
1:A:271:PRO:HG2	1:A:281:THR:CG2	1.96	0.96
1:A:324:GLY:HA2	1:A:329:GLU:OE1	1.73	0.89
1:A:115[B]:ASP:OD2	1:A:118:GLY:HA3	1.73	0.88
2:B:62:ARG:O	2:B:65:LEU:HG	1.74	0.86
2:B:128[A]:ARG:HG3	2:B:128[A]:ARG:NH1	1.88	0.85
2:B:64:VAL:HG13	2:B:69:SER:CB	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ARG:HG3	1:A:297:LEU:HD13	1.61	0.82
1:A:96[A]:ARG:HG3	1:A:96[A]:ARG:NH1	1.93	0.82
2:B:64:VAL:HG22	2:B:69:SER:H	1.44	0.81
2:B:60:VAL:HG13	2:B:64:VAL:HG11	1.60	0.81
1:A:279:THR:O	1:A:283:ILE:HG12	1.80	0.80
1:A:49:TYR:HE2	2:B:42[A]:MET:HE1	1.45	0.78
2:B:128[A]:ARG:CG	2:B:128[A]:ARG:NH1	2.40	0.78
2:B:64:VAL:HG22	2:B:69:SER:N	1.97	0.78
1:A:299[A]:GLU:HA	1:A:299[A]:GLU:OE1	1.87	0.74
2:B:32:ALA:HB2	2:B:94:THR:HG21	1.72	0.72
2:B:205:THR:HG22	2:B:208:ASP:OD2	1.90	0.72
1:A:348:ILE:HG13	1:A:349:PRO:HD2	1.73	0.70
1:A:51:LEU:O	1:A:55:MET:HG2	1.91	0.69
2:B:61:ASP:O	2:B:64:VAL:HB	1.92	0.69
2:B:62:ARG:HG3	2:B:65:LEU:HD21	1.75	0.68
1:A:280:ARG:O	1:A:284:GLU:HG3	1.94	0.68
1:A:451:GLY:O	1:A:452:LEU:HD12	1.92	0.68
1:A:320:VAL:HG13	1:A:397:LEU:HD23	1.74	0.68
1:A:96[A]:ARG:HH11	1:A:96[A]:ARG:HG2	1.59	0.68
1:A:331:SER:HB2	1:A:359:GLU:OE2	1.95	0.67
2:B:340:TRP:CH2	2:B:344:GLU:HG3	2.30	0.67
1:A:315:VAL:HG13	1:A:341:MET:CG	2.27	0.65
1:A:152:ALA:CB	1:A:254[A]:ARG:HD2	2.27	0.65
2:B:31:HIS:NE2	2:B:69:SER:HB2	2.12	0.64
1:A:85:LEU:HG	2:B:1:MET:HE1	1.79	0.64
2:B:64:VAL:HA	2:B:68:GLY:CA	2.22	0.64
2:B:306:PHE:O	2:B:375:GLY:HA2	1.98	0.63
1:A:280:ARG:HG3	1:A:297:LEU:CD1	2.27	0.63
1:A:11:PHE:HD1	1:A:351[A]:MET:HE1	1.62	0.63
1:A:273:PRO:HG3	1:A:282:TRP:CD2	2.33	0.63
2:B:313:ALA:O	2:B:317:LYS:HG3	1.98	0.63
1:A:118:GLY:O	1:A:121:PRO:HD2	1.98	0.62
1:A:308:LEU:HD13	1:A:436:LEU:HD12	1.81	0.62
1:A:157[B]:ARG:HG2	1:A:233:TYR:OH	1.98	0.62
1:A:315:VAL:HG13	1:A:341:MET:HG2	1.82	0.61
2:B:340:TRP:CZ2	2:B:344:GLU:HG3	2.37	0.60
1:A:351[A]:MET:SD	1:A:377:ILE:HG21	2.41	0.60
2:B:64:VAL:HG13	2:B:69:SER:HG	1.65	0.60
2:B:123:ASP:OD2	2:B:137[A]:ARG:NH1	2.34	0.60
2:B:29:ILE:HD11	2:B:58:SER:HB2	1.82	0.60
2:B:64:VAL:CG1	2:B:69:SER:HB3	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:VAL:HA	2:B:64:VAL:HG21	1.85	0.59
1:A:420:GLU:HA	1:A:423:PHE:CE2	2.37	0.58
1:A:11:PHE:CD1	1:A:351[A]:MET:HE1	2.38	0.58
1:A:229:PRO:O	1:A:229:PRO:HD2	2.03	0.58
1:A:97:ASN:N	1:A:98:PRO:CD	2.66	0.58
2:B:95:CYS:HB3	2:B:126:HIS:CE1	2.39	0.58
2:B:172:THR:HG22	2:B:173:THR:O	2.04	0.58
2:B:397:ILE:HB	2:B:401:ASP:HB2	1.85	0.58
2:B:132:LEU:HD23	2:B:224:GLU:HG3	1.84	0.57
1:A:88:LEU:HD13	2:B:3:LEU:HD13	1.85	0.57
1:A:331:SER:CB	1:A:359:GLU:OE2	2.52	0.57
2:B:70:GLN:CB	2:B:107:PHE:CZ	2.81	0.57
1:A:157[B]:ARG:NH1	1:A:157[B]:ARG:CG	2.36	0.57
2:B:64:VAL:HG13	2:B:69:SER:HB3	1.87	0.56
2:B:108:VAL:HG13	2:B:119:VAL:HG12	1.87	0.56
1:A:409:GLU:OE1	1:A:445:ARG:NH2	2.28	0.56
2:B:194:ILE:HG22	2:B:195:GLN:O	2.06	0.55
1:A:42:ILE:O	1:A:106:THR:HB	2.06	0.55
1:A:7:ASN:O	1:A:374:LEU:HD13	2.06	0.55
2:B:358:HIS:ND1	2:B:378[A]:MET:HE2	2.21	0.55
2:B:180:HIS:CD2	2:B:407:ARG:H	2.25	0.54
2:B:31:HIS:NE2	2:B:69:SER:CB	2.71	0.54
2:B:22:SER:HB2	2:B:201:PRO:HB2	1.90	0.54
1:A:232:ARG:HB3	1:A:234:THR:HG22	1.89	0.54
2:B:62:ARG:C	2:B:64:VAL:H	2.14	0.54
1:A:106:THR:HG22	1:A:108:THR:H	1.71	0.54
2:B:400:GLN:H	2:B:400:GLN:CD	2.16	0.54
2:B:63[A]:HIS:CD2	2:B:63[A]:HIS:H	2.26	0.53
2:B:143:VAL:O	2:B:147:ILE:HG12	2.07	0.53
1:A:271:PRO:HG2	1:A:281:THR:HG22	1.85	0.53
2:B:176:PHE:HD1	2:B:397:ILE:HD13	1.74	0.53
1:A:110:GLU:O	1:A:113:LYS:HD3	2.10	0.52
2:B:33:PRO:HD2	2:B:36:ASP:OD2	2.10	0.52
1:A:52:GLN:HA	1:A:59:ILE:HD13	1.91	0.52
2:B:171:ILE:O	2:B:201:PRO:HG2	2.10	0.52
1:A:338:ARG:HD2	1:A:370:MET:HE3	1.90	0.52
1:A:14:GLU:HB2	1:A:381:PRO:HA	1.91	0.51
2:B:377:GLN:OE1	2:B:380:ARG:HD3	2.09	0.51
1:A:196:HIS:CE1	1:A:223:LYS:H	2.28	0.51
1:A:207:ASP:HB3	1:A:208:PRO:HD3	1.92	0.51
1:A:400:THR:O	1:A:417:TRP:HA	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:TRP:HB3	2:B:358:HIS:CD2	2.45	0.51
1:A:354:ARG:HH11	1:A:354:ARG:HG3	1.75	0.50
2:B:62:ARG:O	2:B:65:LEU:CG	2.51	0.50
2:B:64:VAL:CG1	2:B:69:SER:CB	2.83	0.49
2:B:206:VAL:HB	6:B:2033:HOH:O	2.12	0.49
1:A:285:GLN:HE21	1:A:285:GLN:C	2.17	0.49
1:A:22:CYS:SG	1:A:23:PRO:HD2	2.53	0.49
1:A:314:LEU:O	1:A:318:LYS:HD2	2.12	0.49
2:B:73:VAL:O	2:B:77:ILE:HG13	2.13	0.49
2:B:184:GLU:HG2	2:B:410:LEU:O	2.12	0.49
1:A:451:GLY:C	1:A:452:LEU:HD12	2.37	0.48
2:B:232:TYR:CE1	2:B:236:GLU:HG3	2.49	0.48
2:B:67:ARG:HG2	2:B:67:ARG:O	2.13	0.48
2:B:67:ARG:O	2:B:70:GLN:HG2	2.14	0.48
1:A:348:ILE:HG13	1:A:349:PRO:CD	2.41	0.48
1:A:407:PRO:HB2	2:B:52:PHE:CE1	2.49	0.48
2:B:167:ASN:HB2	2:B:218:ASN:OD1	2.13	0.48
1:A:152:ALA:HB2	1:A:254[A]:ARG:HD2	1.96	0.47
1:A:276:PRO:HD3	1:A:432:ALA:CB	2.44	0.47
1:A:334:ARG:HD3	1:A:362:LEU:HD23	1.95	0.47
1:A:229:PRO:O	1:A:229:PRO:CD	2.62	0.47
2:B:14:ILE:O	2:B:18:ARG:HG3	2.15	0.47
2:B:217:PHE:CD1	2:B:263:LEU:HD21	2.50	0.47
1:A:31:TYR:CD1	1:A:31:TYR:C	2.93	0.47
1:A:268:ILE:HG12	1:A:289:THR:HG21	1.98	0.46
2:B:271:ASN:OD1	2:B:273:GLU:HB2	2.16	0.46
1:A:195:PRO:O	1:A:196:HIS:O	2.34	0.46
2:B:60:VAL:HG13	2:B:64:VAL:CG1	2.39	0.46
2:B:76:ASN:N	2:B:76:ASN:HD22	2.12	0.46
2:B:167:ASN:ND2	2:B:215:ALA:HB3	2.32	0.45
2:B:16:THR:HG21	2:B:122:ALA:HB2	1.99	0.45
2:B:17:LEU:HD23	2:B:17:LEU:HA	1.80	0.45
2:B:127:TYR:O	2:B:128[A]:ARG:HD3	2.17	0.45
1:A:330:ILE:CD1	1:A:377:ILE:HD13	2.47	0.45
1:A:276:PRO:HD2	1:A:335:PHE:CE1	2.52	0.45
2:B:68:GLY:O	2:B:70:GLN:N	2.50	0.45
2:B:128[A]:ARG:HH11	2:B:128[A]:ARG:HG2	1.72	0.45
2:B:62:ARG:O	2:B:65:LEU:CD1	2.65	0.44
2:B:218:ASN:HD21	2:B:233:LEU:HD23	1.81	0.44
2:B:241:SER:HB3	6:B:2045:HOH:O	2.17	0.44
1:A:194:HIS:HD2	1:A:221:GLY:HA3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:THR:O	1:A:308:LEU:HG	2.18	0.44
2:B:15:GLY:HA3	2:B:131:GLU:O	2.18	0.43
2:B:398:HIS:HB3	6:B:2094:HOH:O	2.17	0.43
2:B:13:HIS:CD2	2:B:14:ILE:HD12	2.53	0.43
1:A:97:ASN:N	1:A:98:PRO:HD3	2.33	0.43
1:A:330:ILE:HD12	1:A:377:ILE:HD13	1.99	0.43
2:B:49:GLU:HG3	2:B:51:ASP:H	1.83	0.43
2:B:257:ARG:O	2:B:260:GLN:HB3	2.18	0.43
1:A:39:PHE:HD2	1:A:104[B]:ILE:HD11	1.83	0.43
2:B:159:SER:O	2:B:214:GLN:HG2	2.19	0.43
2:B:218:ASN:O	2:B:241:SER:HA	2.19	0.43
1:A:161:SER:O	1:A:162:THR:HB	2.18	0.43
1:A:356:GLN:O	1:A:358:ALA:N	2.52	0.42
1:A:440:THR:O	1:A:441:ARG:C	2.60	0.42
2:B:152[B]:ARG:NH2	6:B:2025:HOH:O	2.51	0.42
1:A:161:SER:O	1:A:162:THR:CB	2.68	0.42
2:B:31:HIS:CE1	2:B:69:SER:HB2	2.54	0.42
1:A:299[A]:GLU:OE1	1:A:299[A]:GLU:CA	2.60	0.42
2:B:64:VAL:C	2:B:66:ALA:N	2.77	0.42
1:A:196:HIS:HA	1:A:197:PRO:HD3	1.97	0.42
2:B:64:VAL:O	2:B:68:GLY:N	2.51	0.41
2:B:107:PHE:N	2:B:107:PHE:CD1	2.85	0.41
2:B:78:ILE:O	2:B:81:ASP:HB3	2.20	0.41
2:B:165:SER:HA	2:B:195:GLN:O	2.20	0.41
2:B:433:HIS:CE1	2:B:437:ILE:HD11	2.55	0.41
1:A:411:ARG:HG3	1:A:458:VAL:HG11	2.01	0.41
2:B:67:ARG:O	2:B:67:ARG:CG	2.69	0.41
2:B:166:VAL:HG22	2:B:167:ASN:N	2.35	0.41
2:B:218:ASN:ND2	2:B:233:LEU:HD23	2.35	0.41
1:A:112:ILE:HG23	2:B:99:ILE:HD12	2.02	0.41
1:A:250:PRO:HA	1:A:272:PHE:CZ	2.56	0.41
2:B:125:ASN:HA	6:B:2017:HOH:O	2.20	0.41
2:B:315:MET:HE1	2:B:418:LEU:HD22	2.02	0.41
1:A:393:LEU:O	1:A:394:GLN:C	2.63	0.41
2:B:64:VAL:HG11	2:B:69:SER:HB3	2.03	0.41
2:B:171:ILE:HG23	2:B:178:ASN:HB3	2.02	0.41
1:A:271:PRO:O	1:A:282:TRP:HD1	2.04	0.41
1:A:331:SER:HB2	1:A:334:ARG:HH21	1.86	0.41
2:B:103:ASP:CG	2:B:106:ASN:HB2	2.47	0.40
2:B:111:ALA:O	2:B:115:THR:HG23	2.21	0.40
1:A:199:LEU:HD21	1:A:201:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:LEU:HA	2:B:3:LEU:HD12	1.87	0.40
2:B:423:TYR:CZ	2:B:427:THR:HG21	2.57	0.40
2:B:167:ASN:OD1	2:B:197:ASN:HB3	2.21	0.40
1:A:108:THR:O	1:A:112:ILE:HG12	2.21	0.40
1:A:416:LYS:NZ	1:A:420:GLU:OE1	2.40	0.40
2:B:166:VAL:CG2	2:B:167:ASN:N	2.85	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	430/460 (94%)	410 (95%)	14 (3%)	6 (1%)	9	13
2	B	450/511 (88%)	423 (94%)	22 (5%)	5 (1%)	11	18
All	All	880/971 (91%)	833 (95%)	36 (4%)	11 (1%)	9	14

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	HIS
1	A	357	ALA
2	B	201	PRO
2	B	396	PRO
1	A	453	GLY
2	B	65	LEU
1	A	143	PHE
1	A	325	ASP
2	B	206	VAL
2	B	439	GLY
1	A	229	PRO

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	367/389 (94%)	339 (92%)	28 (8%)	12	21
2	B	380/420 (90%)	346 (91%)	34 (9%)	9	15
All	All	747/809 (92%)	685 (92%)	62 (8%)	13	17

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	12	GLU
1	A	31	TYR
1	A	57	VAL
1	A	65	TYR
1	A	96[A]	ARG
1	A	96[B]	ARG
1	A	106	THR
1	A	108	THR
1	A	127	ILE
1	A	151	LEU
1	A	154[A]	MET
1	A	154[B]	MET
1	A	162	THR
1	A	248	VAL
1	A	254[A]	ARG
1	A	254[B]	ARG
1	A	285	GLN
1	A	315	VAL
1	A	316	ARG
1	A	320	VAL
1	A	329	GLU
1	A	336	LEU
1	A	342	ARG
1	A	365	GLN
1	A	376	THR
1	A	445	ARG

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Mol	Chain	Res	Type
1	A	454	TRP
2	B	29	ILE
2	B	43	ARG
2	B	46	LEU
2	B	53	THR
2	B	59	ILE
2	B	62	ARG
2	B	63[A]	HIS
2	B	63[B]	HIS
2	B	64	VAL
2	B	71	GLU
2	B	84	GLU
2	B	97	SER
2	B	124	VAL
2	B	128[A]	ARG
2	B	128[B]	ARG
2	B	137[A]	ARG
2	B	137[B]	ARG
2	B	158	THR
2	B	160[A]	LYS
2	B	160[B]	LYS
2	B	206	VAL
2	B	224	GLU
2	B	231	GLN
2	B	233	LEU
2	B	291	ARG
2	B	299	THR
2	B	302	LYS
2	B	367	ARG
2	B	385[A]	ARG
2	B	385[B]	ARG
2	B	400	GLN
2	B	407	ARG
2	B	436	GLU
2	B	437	ILE

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	194	HIS
1	A	212	GLN
1	A	295	GLN

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Mol	Chain	Res	Type
1	A	404	HIS
1	A	427	HIS
2	B	13	HIS
2	B	70	GLN
2	B	76	ASN
2	B	167	ASN
2	B	180	HIS
2	B	197	ASN
2	B	210	GLN
2	B	278	GLN
2	B	279	GLN
2	B	433	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](#)

4 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	$\# Z > 2$
4	MGX	A	1463	-	4,4,4	0.36	0	4,4,4	1.25	1 (25%)
5	SO4	B	1504	-	4,4,4	0.22	0	6,6,6	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	B	1503	-	4,4,4	0.40	0	6,6,6	0.42	0
3	SF4	A	602	1,2	0,12,12	-	-	-		

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	MGX	A	1463	-	-	0/2/2/2	-
3	SF4	A	602	1,2	-	-	0/6/5/5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1463	MGX	CD-NE-CZ	2.44	127.27	121.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	425/460 (92%)	0.25	23 (5%)	31 28	32, 67, 102, 130	9 (2%)
2	B	440/511 (86%)	-0.06	14 (3%)	50 46	33, 54, 128, 276	12 (2%)
All	All	865/971 (89%)	0.09	37 (4%)	40 36	32, 61, 113, 276	21 (2%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	451	GLY	5.4
1	A	6	PRO	4.3
2	B	63[A]	HIS	3.6
2	B	69	SER	3.6
1	A	458	VAL	3.4
2	B	65	LEU	3.3
1	A	368	ALA	3.3
1	A	452	LEU	3.2
1	A	162	THR	3.0
2	B	61	ASP	2.9
2	B	78	ILE	2.9
1	A	456	LYS	2.8
1	A	292	ILE	2.7
1	A	192	GLN	2.7
2	B	101	GLN	2.6
1	A	457	LEU	2.5
1	A	310	ASP	2.5
2	B	433	HIS	2.4
1	A	293	GLN	2.4
2	B	74	VAL	2.4
2	B	277	GLU	2.4
1	A	454	TRP	2.4
1	A	8	ALA	2.3
2	B	151[A]	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	95	ASP	2.2
2	B	385[A]	ARG	2.2
1	A	90	LEU	2.2
2	B	144	GLN	2.1
2	B	105	GLN	2.1
1	A	288	ALA	2.1
1	A	450	ALA	2.1
1	A	459	ALA	2.1
1	A	215	LEU	2.1
1	A	455	GLN	2.0
1	A	137	ASN	2.0
1	A	453	GLY	2.0
2	B	123	ASP	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
5	SO4	B	1503	5/5	0.79	0.12	61,61,117,500	0
4	MGX	A	1463	5/5	0.84	0.22	81,84,89,108	0
5	SO4	B	1504	5/5	0.93	0.08	61,64,179,500	0
3	SF4	A	602	8/8	0.98	0.07	42,46,47,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.