Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:31 AM GMT

PDB ID	:	2XDQ
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

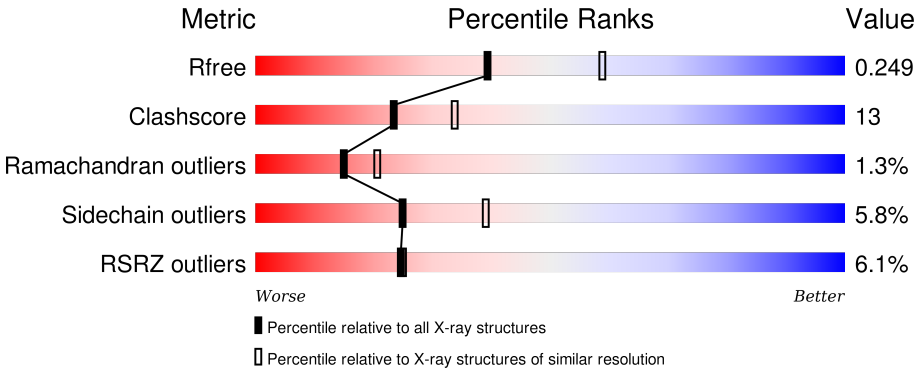
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	10%, 67%, 23%, ·, 8%
2	B	511	%, 61%, 21%, ·, 14%

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	MGX	A	1463	-	-	-	X

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
			Total	C	N	O	S			
1	A	425	3401	2186	579	613	23	0	9	0

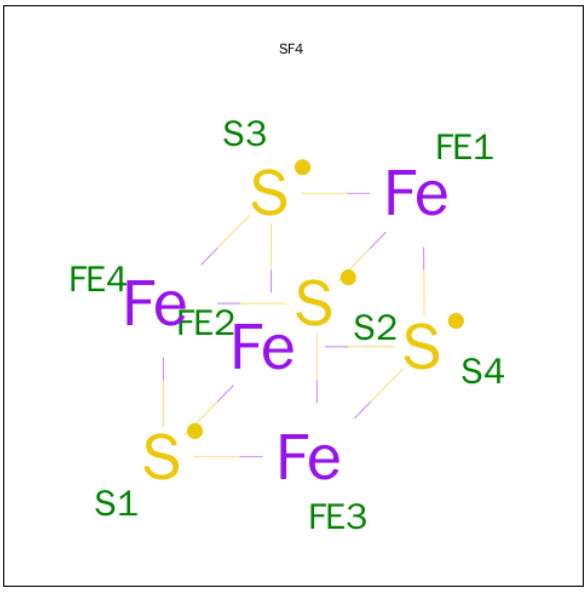
- Molecule 2 is a protein called LIGHT-INDEPENDENT PROTOCHLOROPHYLLIDE REDUCTASE SUBUNIT B.

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

There are 3 discrepancies between the modelled and reference sequences:

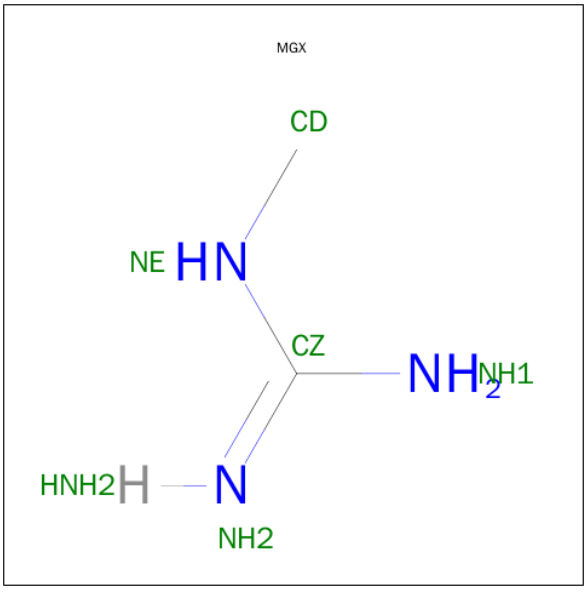
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	ALA	-	EXPRESSION TAG	UNP Q8DGC6
B	-1	ALA	-	EXPRESSION TAG	UNP Q8DGC6
B	0	ALA	-	EXPRESSION TAG	UNP Q8DGC6

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



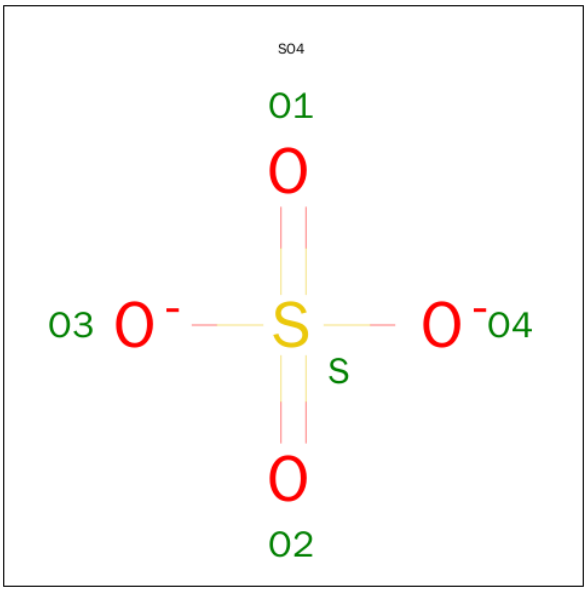
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 8 4 4	0	0

- Molecule 4 is 1-METHYLGUANIDINE (three-letter code: MGX) (formula: $C_2H_7N_3$).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

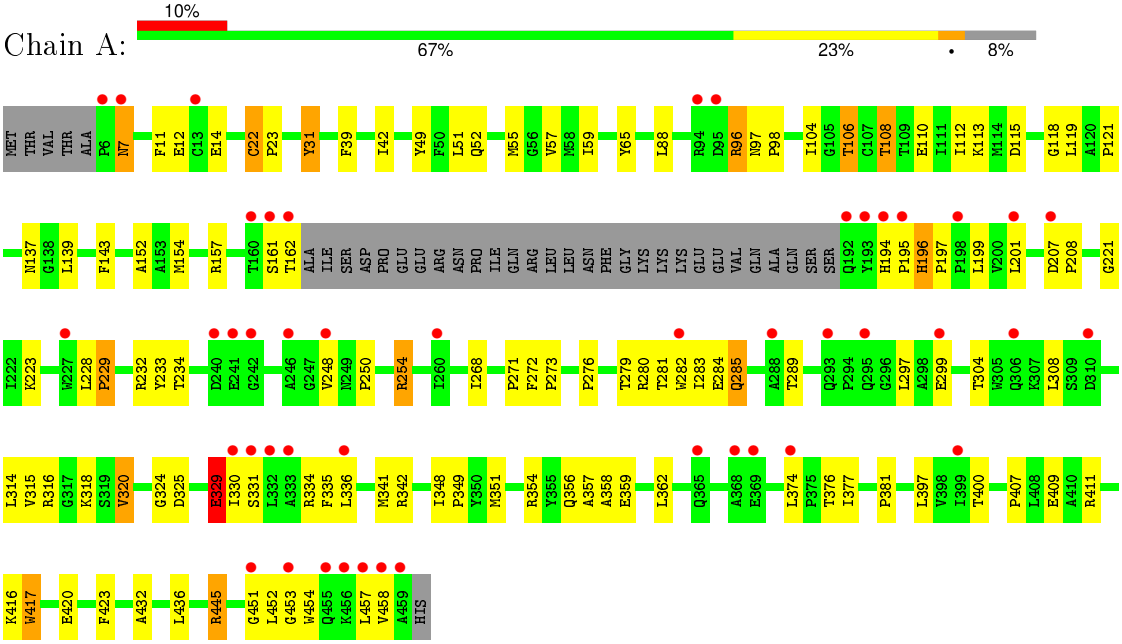
- Molecule 6 is water.

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

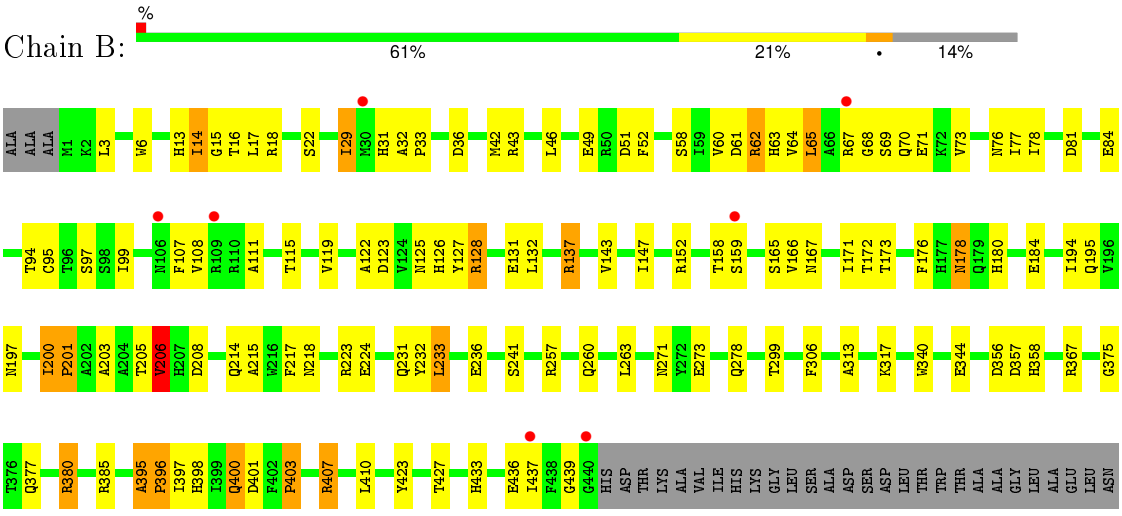
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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




LYS ILE PRO GLY PHE VAL ARG GLY LYS VAL LYS ARG ASN THR GLU LYS PHE ALA ARG GLU GLN GLY ILE SER GLU ILE THR VAL GLU VAL LEU TYR ALA ALA LYS GLU ALA VAL GLY ALA

4 Data and refinement statistics (i)

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 24.75 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.6 (103.65-2.40) 98.7 (24.75-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.34%)	DCC
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 , 52.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 55561 reflections	Xtriage
F_o,F_c correlation	0.95	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: SF4, MGX, 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	0.94	3/3504 (0.1%)	0.88	2/4755 (0.0%)
2	B	0.90	2/3642 (0.1%)	0.90	9/4938 (0.2%)
All	All	0.92	5/7146 (0.1%)	0.89	11/9693 (0.1%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	GLU	CB-CG	7.06	1.65	1.52
2	B	203	ALA	CA-CB	6.90	1.67	1.52
1	A	417	TRP	CB-CG	-6.52	1.38	1.50
2	B	403	PRO	CB-CG	5.02	1.75	1.50
1	A	22	CYS	CB-SG	5.00	1.90	1.82

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	228	LEU	C-N-CD	-20.43	75.66	120.60
2	B	395	ALA	C-N-CD	-18.84	79.15	120.60
2	B	200	ILE	C-N-CD	-15.04	87.50	120.60
1	A	228	LEU	C-N-CA	13.65	179.32	122.00
2	B	396	PRO	CA-N-CD	-6.46	102.45	111.50
2	B	356	ASP	CB-CG-OD1	5.64	123.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	223	ARG	NE-CZ-NH2	-5.50	117.55	120.30
2	B	14	ILE	CG1-CB-CG2	-5.40	99.52	111.40
2	B	395	ALA	C-N-CA	5.40	144.68	122.00
2	B	380	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	B	357	ASP	CB-CG-OD1	5.22	123.00	118.30

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 (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	3401	0	3456	89	0
2	B	3533	0	3553	104	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	186	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 13.

All (186) 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:CG	2:B:403:PRO:CB	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NH1	1:A:157[B]:ARG:HG3	1.64	1.05
1:A:157[B]:ARG:HH11	1:A:157[B]:ARG:CG	1.66	1.05
1:A:96[A]:ARG:CG	1:A:96[A]:ARG:HH11	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:HH11	1:A:157[B]:ARG:HG3	0.85	1.00
1:A:96[A]:ARG:HG3	1:A:96[A]:ARG:HH11	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:NH1	2:B:128[A]:ARG:HG3	1.88	0.85
2:B:64:VAL:HG13	2:B:69:SER:CB	2.08	0.83
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
2:B:128[A]:ARG:NH1	2:B:128[A]:ARG:CG	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:11:PHE:HD1	1:A:351[A]:MET:HE1	1.58	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:HG2	1:A:96[A]:ARG:HH11	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
1:A:11:PHE:CD1	1:A:351[A]:MET:HE1	2.32	0.65
2:B:31:HIS:NE2	2:B:69:SER:HB2	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:229:PRO:HD2	1:A:229:PRO:O	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:397:ILE:HB	2:B:401:ASP:HB2	1.85	0.58
2:B:172:THR:HG22	2:B:173:THR:O	2.04	0.58
2:B:132:LEU:HD23	2:B:224:GLU:HG3	1.84	0.57
1:A:49:TYR:HE2	2:B:42[A]:MET:HE3	1.69	0.57
2:B:70:GLN:CB	2:B:107:PHE:CZ	2.81	0.57
1:A:331:SER:CB	1:A:359:GLU:OE2	2.52	0.57
1:A:88:LEU:HD13	2:B:3:LEU:HD13	1.85	0.57
1:A:157[B]:ARG:CG	1:A:157[B]:ARG:NH1	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:49:TYR:CE2	2:B:42[A]:MET:CE	2.87	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: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
1:A:106:THR:HG22	1:A:108:THR:H	1.71	0.54
2:B:63[A]:HIS:H	2:B:63[A]:HIS:CD2	2.26	0.53
2:B:143:VAL:O	2:B:147:ILE:HG12	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:171:ILE:O	2:B:201:PRO:HG2	2.10	0.52
1:A:52:GLN:HA	1:A:59:ILE:HD13	1.91	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
2:B:6:TRP:HB3	2:B:358:HIS:CD2	2.45	0.51
1:A:49:TYR:CE2	2:B:42[A]:MET:HE1	2.47	0.50
1:A:354:ARG:HG3	1:A:354:ARG:HH11	1.75	0.50
1:A:49:TYR:CE2	2:B:42[A]:MET:HE3	2.44	0.50
2:B:62:ARG:O	2:B:65:LEU:CG	2.51	0.50
2:B:62:ARG:C	2:B:64:VAL:H	2.14	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: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:400:GLN:CD	2:B:400:GLN:H	2.16	0.49
2:B:184:GLU:HG2	2:B:410:LEU:O	2.12	0.49
2:B:232:TYR:CE1	2:B:236:GLU:HG3	2.49	0.48
2:B:67:ARG:O	2:B:67:ARG:HG2	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:334:ARG:HD3	1:A:362:LEU:HD23	1.95	0.47
1:A:276:PRO:HD3	1:A:432:ALA:CB	2.44	0.47
1:A:229:PRO:CD	1:A:229:PRO:O	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	2:B:17:LEU:HD23	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
2:B:128[A]:ARG:HG2	2:B:128[A]:ARG:HH11	1.72	0.45
2:B:68:GLY:O	2:B:70:GLN:N	2.50	0.45
1:A:276:PRO:HD2	1:A:335:PHE:CE1	2.52	0.45
1:A:285:GLN:HE21	1:A:285:GLN:C	2.17	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:304:THR:O	1:A:308:LEU:HG	2.18	0.44
1:A:194:HIS:HD2	1:A:221:GLY:HA3	1.83	0.44
1:A:451:GLY:C	1:A:452:LEU:HD12	2.37	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:330:ILE:HD12	1:A:377:ILE:HD13	1.99	0.43
1:A:97:ASN:N	1:A:98:PRO:HD3	2.33	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
2:B:159:SER:O	2:B:214:GLN:HG2	2.19	0.43
1:A:39:PHE:HD2	1:A:104[B]:ILE:HD11	1.83	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
2:B:152[B]:ARG:NH2	6:B:2025:HOH:O	2.51	0.42
2:B:31:HIS:CE1	2:B:69:SER:HB2	2.54	0.42
1:A:161:SER:O	1:A:162:THR:CB	2.68	0.42
1:A:299[A]:GLU:CA	1:A:299[A]:GLU:OE1	2.60	0.42
1:A:31:TYR:CD1	1:A:31:TYR:C	2.93	0.42
1:A:196:HIS:HA	1:A:197:PRO:HD3	1.97	0.42
2:B:107:PHE:CD1	2:B:107:PHE:N	2.85	0.41
2:B:64:VAL:O	2:B:68:GLY:N	2.51	0.41
2:B:165:SER:HA	2:B:195:GLN:O	2.20	0.41
2:B:78:ILE:O	2:B:81:ASP:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:125:ASN:HA	6:B:2017:HOH:O	2.20	0.41
1:A:250:PRO:HA	1:A:272:PHE:CZ	2.56	0.41
2:B:62:ARG:C	2:B:64:VAL:N	2.74	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:111:ALA:O	2:B:115:THR:HG23	2.21	0.40
2:B:3:LEU:HD12	2:B:3:LEU:HA	1.87	0.40
2:B:423:TYR:CZ	2:B:427:THR:HG21	2.57	0.40
1:A:199:LEU:HD21	1:A:201:LEU:HD21	2.03	0.40
2:B:167:ASN:OD1	2:B:197:ASN:HB3	2.21	0.40
1:A:416:LYS:NZ	1:A:420:GLU:OE1	2.40	0.40
1:A:108:THR:O	1:A:112:ILE:HG12	2.21	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%)	14	19
2	B	450/511 (88%)	423 (94%)	22 (5%)	5 (1%)	17	25
All	All	880/971 (91%)	833 (95%)	36 (4%)	11 (1%)	15	21

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	HIS

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Mol	Chain	Res	Type
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 (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	367/389 (94%)	343 (94%)	24 (6%)	21 33
2	B	380/420 (90%)	356 (94%)	24 (6%)	22 35
All	All	747/809 (92%)	699 (94%)	48 (6%)	25 34

All (48) 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	154[A]	MET
1	A	154[B]	MET
1	A	248	VAL
1	A	254[A]	ARG

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Mol	Chain	Res	Type
1	A	254[B]	ARG
1	A	285	GLN
1	A	316	ARG
1	A	320	VAL
1	A	329	GLU
1	A	336	LEU
1	A	342	ARG
1	A	376	THR
1	A	445	ARG
1	A	454	TRP
1	A	457	LEU
2	B	29	ILE
2	B	43	ARG
2	B	46	LEU
2	B	62	ARG
2	B	71	GLU
2	B	84	GLU
2	B	97	SER
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	178	ASN
2	B	206	VAL
2	B	231	GLN
2	B	233	LEU
2	B	278	GLN
2	B	299	THR
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	HIS
1	A	295	GLN
2	B	13	HIS

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Mol	Chain	Res	Type
2	B	70	GLN
2	B	76	ASN
2	B	180	HIS
2	B	210	GLN
2	B	278	GLN
2	B	433	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	-	1,4,4	0.10	0	0,4,4	0.00	-
3	SF4	A	602	1,2	0,12,12	0.00	-	0,24,24	0.00	-
5	SO4	B	1503	-	4,4,4	0.30	0	6,6,6	0.32	0
5	SO4	B	1504	-	4,4,4	0.42	0	6,6,6	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MGX	A	1463	-	-	0/0/2/2	0/0/0/0
3	SF4	A	602	1,2	-	0/0/48/48	0/6/5/5
5	SO4	B	1503	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1504	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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, 95^{th} 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%)	0.34	46 (10%) 8 8	45, 68, 102, 130	0
2	B	440/511 (86%)	-0.20	7 (1%) 74 74	34, 55, 128, 276	0
All	All	865/971 (89%)	0.06	53 (6%) 25 25	34, 62, 114, 276	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	451	GLY	7.3
1	A	6	PRO	6.0
1	A	459	ALA	5.3
1	A	162	THR	5.3
1	A	455	GLN	4.9
1	A	458	VAL	4.6
1	A	194	HIS	4.5
1	A	368	ALA	4.5
1	A	456	LYS	4.4
2	B	67	ARG	4.4
1	A	332	LEU	4.2
1	A	457	LEU	4.1
1	A	201	LEU	4.0
1	A	248	VAL	3.9
1	A	94	ARG	3.8
1	A	299[A]	GLU	3.7
1	A	330	ILE	3.6
1	A	161	SER	3.6
1	A	293	GLN	3.5
1	A	242	GLY	3.5
2	B	106	ASN	3.4
1	A	195	PRO	3.4
2	B	109	ARG	3.3
1	A	241	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	374	LEU	3.0
1	A	453	GLY	3.0
1	A	192	GLN	3.0
1	A	7	ASN	3.0
1	A	288	ALA	2.9
1	A	193	TYR	2.8
1	A	310	ASP	2.6
1	A	246	ALA	2.6
2	B	440	GLY	2.6
2	B	30	MET	2.6
1	A	306	GLN	2.5
1	A	160	THR	2.5
1	A	13	CYS	2.5
1	A	260	ILE	2.4
1	A	399	ILE	2.4
2	B	159	SER	2.4
1	A	295	GLN	2.4
1	A	333	ALA	2.4
1	A	331	SER	2.3
1	A	207	ASP	2.3
1	A	365	GLN	2.2
1	A	282	TRP	2.2
1	A	240	ASP	2.2
1	A	198	PRO	2.1
1	A	336	LEU	2.1
1	A	369	GLU	2.1
1	A	95	ASP	2.1
1	A	227	TRP	2.1
2	B	437	ILE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	MGX	A	1463	5/5	0.93	0.20	7.36	81,84,89,108	0
3	SF4	A	602	8/8	0.99	0.05	-2.64	42,46,47,50	0
5	SO4	B	1504	5/5	0.90	0.23	-	61,64,179,500	0
5	SO4	B	1503	5/5	0.76	0.49	-	61,61,117,500	0

6.5 Other polymers

There are no such residues in this entry.