Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:20 AM GMT

PDB ID	:	3AES
Title	:	Structure of the light-independent protochlorophyllide reductase catalyzing a key reduction for greening in the dark
Authors	:	Muraki, N.; Nomata, J.; Shiba, T.; Fujita, Y.; Kurisu, G.
Deposited on	:	2010-02-10
Resolution	:	2.50 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:

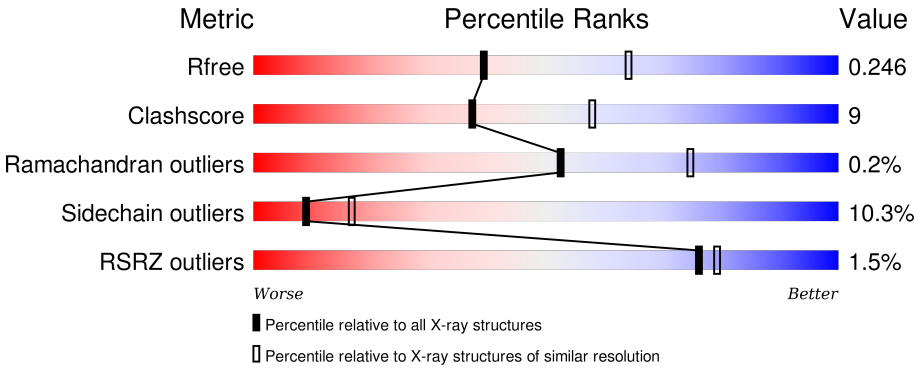
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	436	3% 74% 17% • 5%
1	C	436	% 77% 15% • 5%
2	B	525	% 64% 13% • 20%
2	D	525	% 65% 13% • 20%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13131 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	415	Total	C	N	O	S	Se	0	1	0
			3178	2018	560	585	8	7			
1	C	414	Total	C	N	O	S	Se	0	1	0
			3174	2016	559	584	8	7			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MSE	-	EXPRESSION TAG	UNP P26164
A	-10	ALA	-	EXPRESSION TAG	UNP P26164
A	-9	SER	-	EXPRESSION TAG	UNP P26164
A	-8	TRP	-	EXPRESSION TAG	UNP P26164
A	-7	SER	-	EXPRESSION TAG	UNP P26164
A	-6	HIS	-	EXPRESSION TAG	UNP P26164
A	-5	PRO	-	EXPRESSION TAG	UNP P26164
A	-4	GLN	-	EXPRESSION TAG	UNP P26164
A	-3	PHE	-	EXPRESSION TAG	UNP P26164
A	-2	GLU	-	EXPRESSION TAG	UNP P26164
A	-1	LYS	-	EXPRESSION TAG	UNP P26164
A	0	GLY	-	EXPRESSION TAG	UNP P26164
A	1	ALA	-	EXPRESSION TAG	UNP P26164
C	-11	MSE	-	EXPRESSION TAG	UNP P26164
C	-10	ALA	-	EXPRESSION TAG	UNP P26164
C	-9	SER	-	EXPRESSION TAG	UNP P26164
C	-8	TRP	-	EXPRESSION TAG	UNP P26164
C	-7	SER	-	EXPRESSION TAG	UNP P26164
C	-6	HIS	-	EXPRESSION TAG	UNP P26164
C	-5	PRO	-	EXPRESSION TAG	UNP P26164
C	-4	GLN	-	EXPRESSION TAG	UNP P26164
C	-3	PHE	-	EXPRESSION TAG	UNP P26164
C	-2	GLU	-	EXPRESSION TAG	UNP P26164
C	-1	LYS	-	EXPRESSION TAG	UNP P26164
C	0	GLY	-	EXPRESSION TAG	UNP P26164

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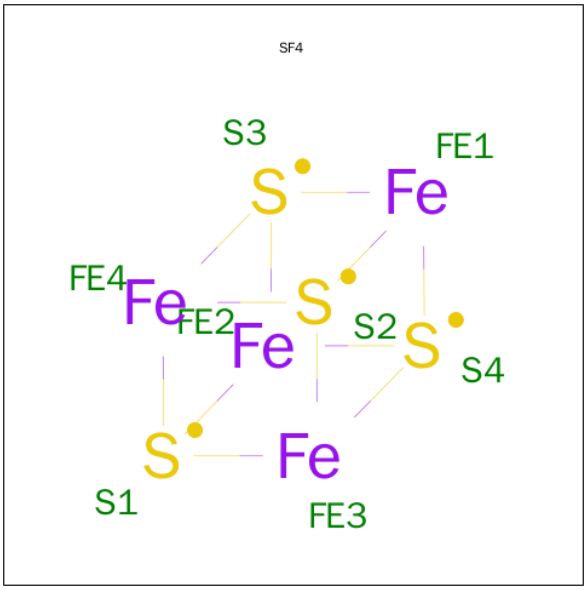
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	ALA	-	EXPRESSION TAG	UNP P26164

- Molecule 2 is a protein called Light-independent protochlorophyllide reductase subunit B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	Se	0	1	0
			3228	2054	558	594	6	16			
2	D	421	Total	C	N	O	S	Se	0	0	0
			3228	2053	558	596	6	15			

- 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		0	0
			8	4	4			
3	C	1	Total	Fe	S		0	0
			8	4	4			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	68	Total	O	0	0
			68	68		
4	B	73	Total	O	0	0
			73	73		

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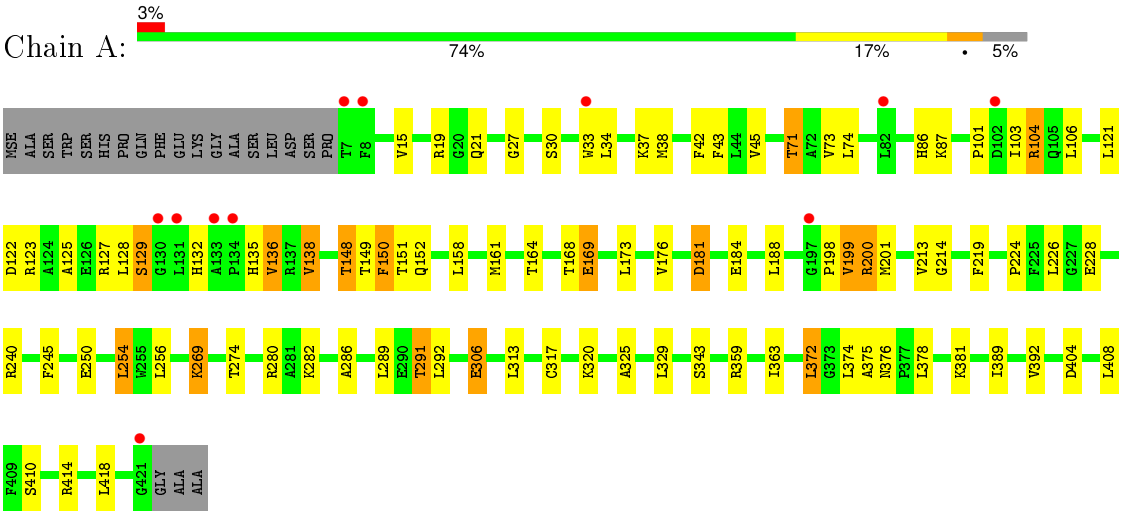
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	86	Total O 86 86	0	0
4	D	80	Total O 80 80	0	0

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.

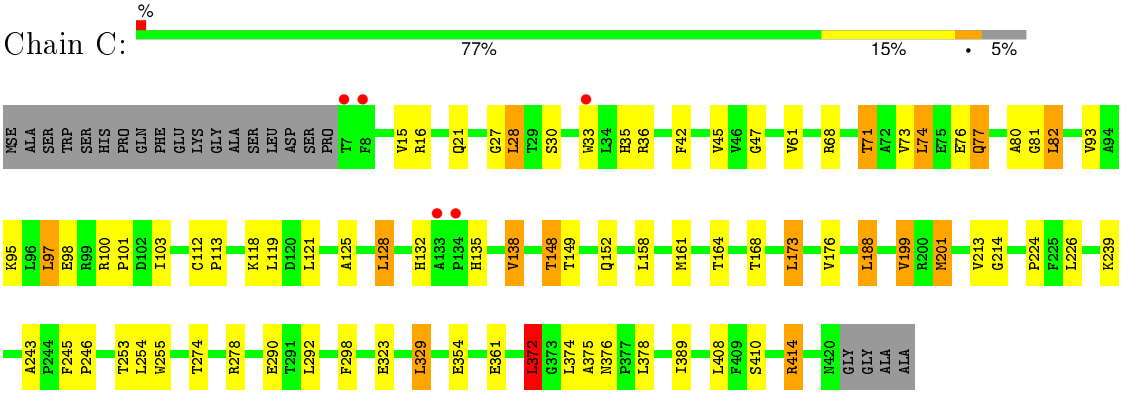
- Molecule 1: Light-independent protochlorophyllide reductase subunit N

Chain A:



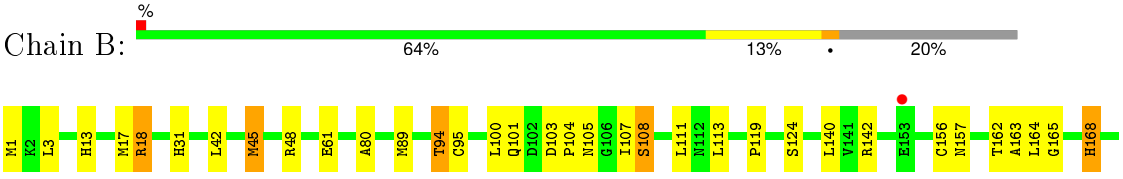
- Molecule 1: Light-independent protochlorophyllide reductase subunit N

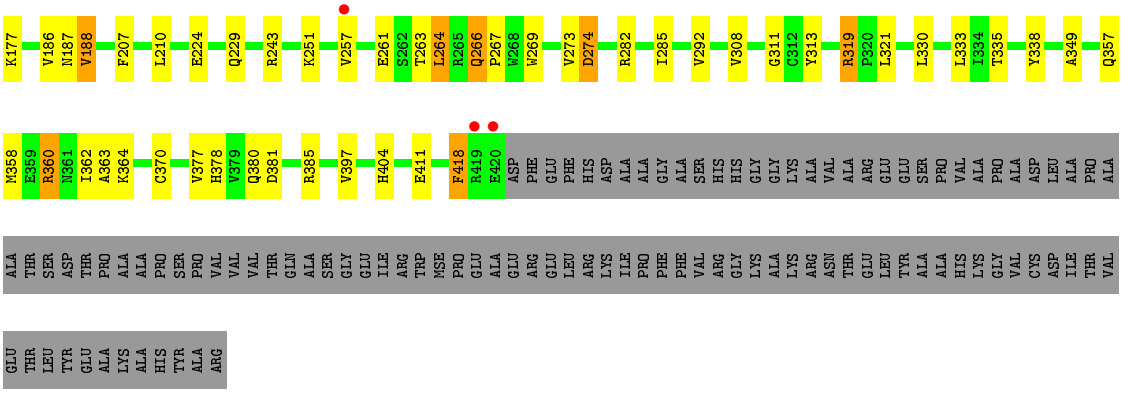
Chain C:



- Molecule 2: Light-independent protochlorophyllide reductase subunit B

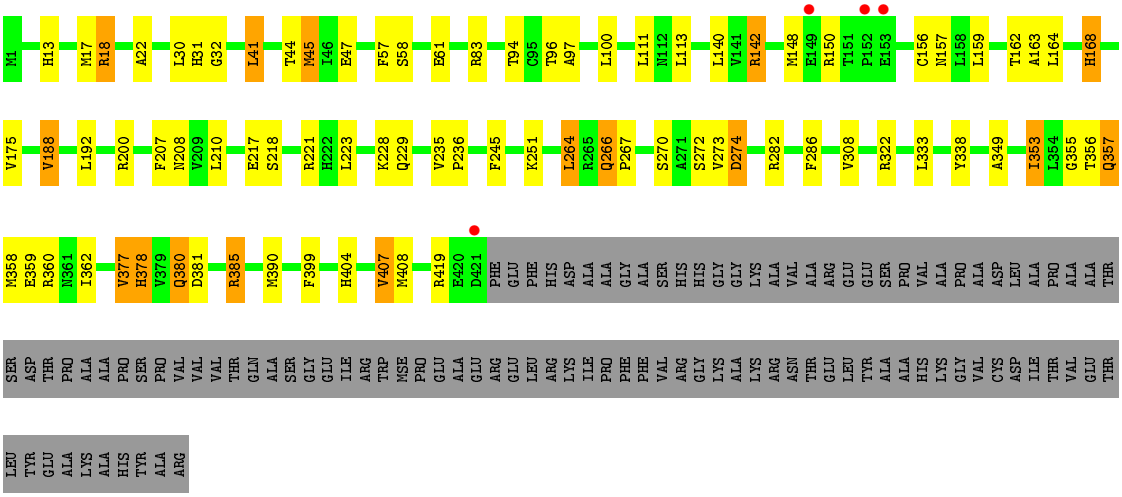
Chain B:





- Molecule 2: Light-independent protochlorophyllide reductase subunit B

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.30Å 80.92Å 176.24Å 90.00° 100.87° 90.00°	Depositor
Resolution (Å)	34.75 – 2.50 34.74 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.75-2.50) 99.9 (34.74-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.208 , 0.248 0.208 , 0.246	Depositor DCC
R_{free} test set	3918 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	40.6	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 34.5	EDS
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	2 of 78115 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13131	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.09% 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

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	0.46	0/3236	0.64	0/4384
1	C	0.48	0/3232	0.64	2/4379 (0.0%)
2	B	0.48	0/3285	0.64	0/4447
2	D	0.49	0/3285	0.63	1/4448 (0.0%)
All	All	0.48	0/13038	0.64	3/17658 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	41	LEU	CA-CB-CG	5.96	129.01	115.30
1	C	329	LEU	CA-CB-CG	5.61	128.19	115.30
1	C	372	LEU	CA-CB-CG	5.23	127.33	115.30

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	3178	0	3208	62	0
1	C	3174	0	3205	46	0
2	B	3228	0	3253	68	0
2	D	3228	0	3249	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	8	0	0	0	0
3	C	8	0	0	1	0
4	A	68	0	0	2	0
4	B	73	0	0	1	0
4	C	86	0	0	2	0
4	D	80	0	0	3	0
All	All	13131	0	12915	240	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (240) 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:188:LEU:HD11	1:A:201:MSE:CE	1.92	1.00
2:B:377:VAL:CG1	2:B:381:ASP:HB2	1.92	0.99
1:A:34:LEU:HG	1:A:38:MSE:CE	1.92	0.98
2:D:338:TYR:CD1	2:D:358:MSE:HE2	1.99	0.98
2:D:13:HIS:HD2	2:D:17:MSE:HE3	1.27	0.98
2:B:358:MSE:HE3	2:B:362:ILE:HG13	1.41	0.97
2:D:175:VAL:CG2	2:D:390:MSE:HE2	1.96	0.96
2:B:377:VAL:HG13	2:B:381:ASP:HB2	1.48	0.94
2:D:13:HIS:HD2	2:D:17:MSE:CE	1.79	0.93
2:B:45:MSE:HA	2:B:45:MSE:HE3	1.51	0.90
2:D:13:HIS:CD2	2:D:17:MSE:HE3	2.07	0.90
1:A:34:LEU:HG	1:A:38:MSE:HE2	1.55	0.89
2:D:356:THR:HG22	2:D:358:MSE:H	1.37	0.88
1:A:200:ARG:CG	1:A:200:ARG:HH11	1.86	0.88
1:A:306:GLU:HG3	1:A:325:ALA:O	1.71	0.88
2:D:162:THR:H	2:D:168:HIS:HD2	1.16	0.88
2:D:338:TYR:HD1	2:D:358:MSE:HE2	1.37	0.86
2:D:356:THR:HB	2:D:359:GLU:OE2	1.74	0.86
2:D:377:VAL:CG1	2:D:381:ASP:HB2	2.05	0.86
1:C:95:LYS:HB2	4:C:497:HOH:O	1.76	0.85
1:A:200:ARG:HG2	1:A:200:ARG:HH11	1.43	0.84
2:D:175:VAL:CG2	2:D:390:MSE:CE	2.55	0.84
2:D:13:HIS:CD2	2:D:17:MSE:CE	2.62	0.83
1:A:34:LEU:HG	1:A:38:MSE:HE1	1.61	0.82
1:A:19:ARG:HG2	1:A:19:ARG:HH11	1.43	0.81
2:D:377:VAL:HG13	2:D:381:ASP:HB2	1.62	0.81
1:C:149:THR:H	1:C:152:GLN:HE21	1.27	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:LEU:HA	1:C:161:MSE:HE3	1.61	0.81
2:D:18:ARG:HH11	2:D:18:ARG:HG2	1.46	0.80
2:D:142:ARG:HG2	2:D:142:ARG:HH11	1.45	0.79
1:A:149:THR:H	1:A:152:GLN:HE21	1.31	0.79
2:D:322:ARG:HD3	4:D:565:HOH:O	1.83	0.78
2:B:273:VAL:H	1:C:376:ASN:HD21	1.31	0.78
1:C:188:LEU:HD11	1:C:201:MSE:HE1	1.65	0.77
2:B:162:THR:H	2:B:168:HIS:HD2	1.32	0.76
1:A:188:LEU:HD11	1:A:201:MSE:HE1	1.64	0.76
2:D:148:MSE:HE1	2:D:200:ARG:O	1.85	0.75
1:A:188:LEU:HD11	1:A:201:MSE:HE3	1.67	0.75
2:B:45:MSE:HA	2:B:45:MSE:CE	2.17	0.75
2:D:175:VAL:HG22	2:D:390:MSE:HE2	1.66	0.75
2:B:377:VAL:HG11	2:B:381:ASP:HB2	1.66	0.74
2:B:418:PHE:HB3	1:C:36:ARG:NH1	2.03	0.73
2:B:18:ARG:HD2	2:B:164:LEU:HB2	1.71	0.73
2:D:358:MSE:HE3	2:D:362:ILE:CG1	2.19	0.73
2:D:378:HIS:HB2	4:D:601:HOH:O	1.90	0.71
2:D:18:ARG:HG2	2:D:163:ALA:O	1.90	0.71
2:B:357:GLN:OE1	2:B:360:ARG:NH1	2.22	0.71
2:B:13:HIS:HD2	2:B:17:MSE:CE	2.03	0.71
2:D:358:MSE:HE3	2:D:362:ILE:HG13	1.73	0.71
1:C:27:GLY:HA3	1:C:148:THR:CG2	2.20	0.71
2:D:353:ILE:HD11	2:D:359:GLU:HB3	1.73	0.69
2:D:377:VAL:HG11	2:D:381:ASP:HB2	1.76	0.68
2:D:286:PHE:O	2:D:355:GLY:HA2	1.93	0.68
2:B:274:ASP:HB2	2:D:45:MSE:HE2	1.76	0.67
2:D:45:MSE:HA	2:D:45:MSE:HE3	1.77	0.67
2:D:175:VAL:HG21	2:D:390:MSE:HE1	1.76	0.66
1:A:158:LEU:HD23	1:A:161:MSE:HE3	1.76	0.66
2:B:13:HIS:CD2	2:B:17:MSE:CE	2.79	0.66
2:B:377:VAL:HG11	2:B:381:ASP:CB	2.26	0.65
2:B:103:ASP:O	2:B:107:ILE:HG12	1.97	0.64
2:B:13:HIS:CD2	2:B:17:MSE:HE3	2.33	0.64
1:A:132:HIS:HB3	1:A:136:VAL:HG13	1.79	0.64
1:A:376:ASN:OD1	2:B:45:MSE:HE1	1.99	0.63
2:B:358:MSE:CE	2:B:362:ILE:HG13	2.21	0.63
2:D:236:PRO:HG2	2:D:390:MSE:HE3	1.80	0.63
1:C:45:VAL:HB	1:C:71:THR:HB	1.78	0.63
2:D:175:VAL:HG21	2:D:390:MSE:CE	2.27	0.63
1:C:372:LEU:HD22	1:C:389:ILE:HD13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ASN:HD21	2:D:273:VAL:H	1.47	0.62
1:A:37:LYS:NZ	1:A:184:GLU:OE1	2.32	0.62
2:B:378:HIS:CE1	2:B:380:GLN:HB3	2.34	0.62
2:B:157:ASN:HD22	2:B:188:VAL:H	1.48	0.62
1:C:16:ARG:NH1	4:C:508:HOH:O	2.34	0.61
2:B:13:HIS:HD2	2:B:17:MSE:HE3	1.65	0.61
2:D:96:THR:HG23	4:D:529:HOH:O	1.98	0.61
1:A:176:VAL:HG12	1:A:226:LEU:HD13	1.83	0.61
1:A:71:THR:HG23	4:B:583:HOH:O	1.99	0.60
2:B:264:LEU:HD22	2:B:267:PRO:HD3	1.84	0.60
1:A:38:MSE:CE	1:A:43:PHE:HZ	2.15	0.60
2:D:356:THR:HG22	2:D:358:MSE:N	2.13	0.59
1:C:30:SER:HA	1:C:33[B]:TRP:CZ3	2.37	0.59
1:C:27:GLY:HA3	1:C:148:THR:HG21	1.83	0.59
1:A:42:PHE:HB2	1:A:103:ILE:HG12	1.83	0.59
1:A:381:LYS:HD3	4:A:448:HOH:O	2.02	0.58
1:A:38:MSE:HE1	1:A:43:PHE:HZ	1.69	0.58
2:B:105:ASN:HD22	2:B:119:PRO:HG3	1.68	0.58
1:A:19:ARG:HG2	1:A:19:ARG:NH1	2.18	0.57
1:C:112:CYS:HB2	2:D:96:THR:HG21	1.87	0.57
1:A:101:PRO:O	1:A:135:HIS:HE1	1.88	0.57
2:D:236:PRO:CG	2:D:390:MSE:HE3	2.34	0.57
2:B:411:GLU:HG3	1:C:61:VAL:HG11	1.87	0.57
1:A:27:GLY:HA3	1:A:148:THR:CG2	2.34	0.57
1:C:246:PRO:HD3	1:C:255:TRP:CD1	2.40	0.57
1:A:125:ALA:O	1:A:129:SER:HB2	2.04	0.56
2:D:162:THR:H	2:D:168:HIS:CD2	2.08	0.56
1:C:101:PRO:O	1:C:135:HIS:HE1	1.88	0.56
2:D:377:VAL:HG11	2:D:381:ASP:CB	2.36	0.56
2:D:142:ARG:HG2	2:D:142:ARG:NH1	2.20	0.56
2:D:22:ALA:HB1	2:D:192:LEU:HA	1.88	0.55
1:A:30:SER:HA	1:A:33[B]:TRP:CZ3	2.41	0.55
1:A:372:LEU:HD22	1:A:389:ILE:HD13	1.88	0.55
2:D:32:GLY:HA2	2:D:94:THR:HG21	1.88	0.55
2:D:175:VAL:HG22	2:D:390:MSE:CE	2.29	0.55
1:C:149:THR:N	1:C:152:GLN:HE21	2.01	0.55
1:A:150:PHE:CE2	1:A:392:VAL:HG21	2.42	0.54
1:A:375:ALA:HB1	2:D:273:VAL:HG21	1.89	0.54
2:B:105:ASN:ND2	2:B:119:PRO:HG3	2.22	0.54
2:D:13:HIS:O	2:D:17:MSE:HG3	2.08	0.54
1:A:200:ARG:NH1	1:A:200:ARG:HG2	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:ILE:H	1:A:389:ILE:HD12	1.73	0.53
1:A:200:ARG:HG3	1:A:200:ARG:HH11	1.71	0.53
1:A:376:ASN:OD1	2:B:45:MSE:CE	2.56	0.53
1:A:359:ARG:O	1:A:363:ILE:HD12	2.09	0.53
1:A:200:ARG:NH1	1:A:200:ARG:CG	2.57	0.53
2:D:18:ARG:NH1	2:D:18:ARG:HG2	2.18	0.53
2:D:356:THR:CG2	2:D:357:GLN:N	2.71	0.53
2:D:45:MSE:HA	2:D:45:MSE:CE	2.39	0.53
1:A:33[B]:TRP:CH2	1:A:151:THR:HG22	2.43	0.53
1:C:35:HIS:O	1:C:68:ARG:NH2	2.42	0.52
2:B:380:GLN:NE2	2:D:404:HIS:ND1	2.56	0.52
2:B:13:HIS:HD2	2:B:17:MSE:HE2	1.75	0.52
1:A:158:LEU:HA	1:A:161:MSE:HE3	1.91	0.52
2:D:18:ARG:NH1	2:D:163:ALA:O	2.42	0.52
2:D:270:SER:HB3	2:D:399:PHE:HE1	1.75	0.52
1:A:291:THR:HG21	1:A:414:ARG:HH11	1.74	0.52
1:C:372:LEU:O	2:D:44:THR:HG21	2.09	0.51
1:A:410:SER:O	1:A:414:ARG:HG3	2.10	0.51
1:A:168:THR:O	1:A:214:GLY:HA3	2.11	0.51
1:A:219:PHE:CE2	1:A:240:ARG:HG3	2.45	0.51
1:A:86:HIS:ND1	1:A:127:ARG:NH2	2.58	0.51
2:B:157:ASN:ND2	2:B:188:VAL:H	2.08	0.51
1:A:169:GLU:O	1:A:169:GLU:HG3	2.11	0.51
2:D:175:VAL:CG2	2:D:390:MSE:HE1	2.34	0.50
2:B:18:ARG:CD	2:B:164:LEU:HB2	2.38	0.50
1:C:42:PHE:HB2	1:C:103:ILE:HG12	1.94	0.50
2:B:18:ARG:HG3	2:B:163:ALA:O	2.11	0.49
2:B:313:TYR:HA	2:B:335:THR:O	2.12	0.49
1:A:106:LEU:HB3	1:A:138:VAL:HB	1.94	0.49
2:D:236:PRO:HD2	2:D:390:MSE:HE3	1.95	0.49
1:A:250:GLU:HG2	1:A:254:LEU:HD22	1.94	0.49
1:A:199:VAL:HG22	1:A:201:MSE:HE1	1.95	0.48
2:B:156:CYS:HB3	2:B:207:PHE:CE2	2.49	0.48
2:D:157:ASN:HD22	2:D:188:VAL:H	1.61	0.48
1:A:37:LYS:HE3	1:A:181:ASP:OD1	2.13	0.48
1:C:125:ALA:HA	1:C:138:VAL:HG22	1.94	0.48
1:C:253:THR:OG1	1:C:278:ARG:HD3	2.13	0.48
2:D:378:HIS:CE1	2:D:380:GLN:HB3	2.49	0.48
2:D:157:ASN:HB2	2:D:208:ASN:OD1	2.13	0.48
2:B:380:GLN:HE22	2:D:404:HIS:HB2	1.78	0.48
2:D:266:GLN:HE21	2:D:267:PRO:N	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:404:HIS:ND1	2:D:380:GLN:NE2	2.61	0.48
2:D:31:HIS:HD2	2:D:58:SER:OG	1.97	0.48
1:C:298:PHE:CE1	1:C:323:GLU:HB3	2.48	0.48
1:A:200:ARG:C	1:A:201:MSE:HE2	2.34	0.47
2:D:357:GLN:CD	2:D:378:HIS:HB3	2.34	0.47
2:B:364:LYS:HA	2:B:364:LYS:HD2	1.78	0.47
1:A:73:VAL:O	2:B:1:MSE:HA	2.15	0.47
1:A:38:MSE:CE	1:A:43:PHE:CZ	2.97	0.47
1:C:389:ILE:H	1:C:389:ILE:HD12	1.80	0.47
1:C:27:GLY:CA	1:C:148:THR:CG2	2.92	0.47
1:A:269:LYS:NZ	4:A:493:HOH:O	2.47	0.47
1:C:168:THR:O	1:C:214:GLY:HA3	2.15	0.47
2:D:236:PRO:HG3	2:D:245:PHE:CG	2.50	0.47
2:D:217:GLU:OE2	2:D:221:ARG:NH2	2.48	0.47
2:B:104:PRO:O	2:B:108:SER:HB3	2.15	0.46
2:D:407:VAL:HG23	2:D:408:MSE:HE2	1.98	0.46
1:C:113:PRO:HG3	2:D:96:THR:HG22	1.96	0.46
2:D:157:ASN:ND2	2:D:188:VAL:HG13	2.30	0.46
2:D:378:HIS:HE1	2:D:380:GLN:HB3	1.79	0.46
2:B:45:MSE:HE2	2:D:274:ASP:OD2	2.15	0.46
2:B:377:VAL:CG1	2:B:381:ASP:CB	2.77	0.46
2:D:94:THR:HG23	2:D:97:ALA:H	1.81	0.46
1:A:224:PRO:HA	1:A:245:PHE:CZ	2.50	0.46
2:D:175:VAL:HG23	2:D:390:MSE:HE2	1.93	0.46
1:C:243:ALA:HB1	1:C:255:TRP:HA	1.98	0.46
2:B:282:ARG:NH1	2:B:349:ALA:O	2.49	0.46
2:B:397:VAL:HG22	2:D:385:ARG:HD3	1.98	0.45
2:B:162:THR:H	2:B:168:HIS:CD2	2.22	0.45
2:D:156:CYS:HB3	2:D:207:PHE:CE2	2.51	0.45
2:B:18:ARG:HD2	2:B:163:ALA:O	2.15	0.45
1:C:112:CYS:HB2	1:C:113:PRO:HD3	1.99	0.45
1:A:104:ARG:HH21	1:A:135:HIS:HD2	1.64	0.45
1:C:97:LEU:HD23	1:C:132:HIS:CD2	2.52	0.45
1:C:158:LEU:HD23	1:C:161:MSE:HE1	1.99	0.44
1:C:77:GLN:H	1:C:77:GLN:HG3	1.51	0.44
2:B:94:THR:HG23	2:B:95:CYS:N	2.32	0.44
2:B:319:ARG:HG2	2:B:319:ARG:H	1.60	0.44
2:D:47:GLU:HG3	2:D:164:LEU:HD23	1.99	0.44
1:C:27:GLY:HA3	1:C:148:THR:HG23	1.96	0.44
2:D:235:VAL:HA	2:D:236:PRO:HD3	1.80	0.44
1:C:410:SER:O	1:C:414:ARG:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:GLN:HE21	2:B:267:PRO:N	2.16	0.44
2:B:338:TYR:HB2	2:B:358:MSE:HG2	1.98	0.43
1:A:101:PRO:O	1:A:135:HIS:CE1	2.71	0.43
1:A:38:MSE:HE1	1:A:43:PHE:CZ	2.49	0.43
2:B:31:HIS:O	2:B:94:THR:HB	2.18	0.43
2:B:80:ALA:HB3	2:B:89:MSE:HE1	1.99	0.43
2:B:45:MSE:HE2	2:D:274:ASP:CG	2.39	0.43
2:B:273:VAL:HG21	1:C:375:ALA:HB1	2.00	0.43
1:A:27:GLY:HA3	1:A:148:THR:HG21	1.99	0.43
1:A:27:GLY:HA3	1:A:148:THR:HG23	2.01	0.43
1:C:376:ASN:HB2	2:D:44:THR:HG23	2.00	0.43
2:D:94:THR:CG2	2:D:97:ALA:H	2.32	0.43
2:D:270:SER:HB3	2:D:399:PHE:CE1	2.53	0.43
2:D:223:LEU:HB3	2:D:229:GLN:HE21	1.84	0.43
1:C:28:LEU:HD22	3:C:425:SF4:S2	2.60	0.42
1:C:224:PRO:HA	1:C:245:PHE:CZ	2.54	0.42
2:B:363:ALA:CB	2:B:370:CYS:HB2	2.49	0.42
1:C:173:LEU:HB3	1:C:199:VAL:HB	2.01	0.42
2:B:165:GLY:HA3	2:B:168:HIS:CD2	2.54	0.42
1:A:286:ALA:HA	1:A:289:LEU:HG	2.00	0.42
1:A:291:THR:HG21	1:A:414:ARG:NH1	2.34	0.42
1:C:176:VAL:HG12	1:C:226:LEU:HD13	2.01	0.42
2:D:282:ARG:NH1	2:D:349:ALA:O	2.52	0.42
2:D:30:LEU:O	2:D:57:PHE:HA	2.19	0.42
2:D:264:LEU:HD22	2:D:267:PRO:HD3	2.02	0.42
1:C:47:GLY:O	1:C:74:LEU:HD22	2.20	0.42
2:B:311:GLY:HA2	2:B:321:LEU:HD21	2.02	0.42
2:B:243:ARG:HH22	2:B:261:GLU:CD	2.23	0.42
2:B:13:HIS:O	2:B:17:MSE:HG3	2.20	0.42
2:B:380:GLN:CD	2:D:404:HIS:ND1	2.73	0.42
2:B:95:CYS:HB3	2:B:124:SER:OG	2.20	0.42
2:B:165:GLY:HA3	2:B:168:HIS:CG	2.54	0.41
2:D:236:PRO:CD	2:D:390:MSE:HE3	2.50	0.41
2:B:103:ASP:HA	2:B:104:PRO:HD2	1.97	0.41
2:B:378:HIS:CE1	2:B:380:GLN:CB	3.02	0.41
1:C:354:GLU:HB3	2:D:83:ARG:CZ	2.50	0.41
2:D:13:HIS:HD2	2:D:17:MSE:HE2	1.77	0.41
2:B:48:ARG:HD2	2:D:272:SER:OG	2.19	0.41
1:C:290:GLU:OE2	1:C:290:GLU:HA	2.20	0.41
1:C:93:VAL:HG11	1:C:128:LEU:HG	2.02	0.41
2:B:224:GLU:HA	2:B:229:GLN:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:VAL:HB	1:A:71:THR:HB	2.03	0.41
2:B:285:ILE:HG22	2:B:292:VAL:HG13	2.03	0.41
2:B:358:MSE:CE	2:B:362:ILE:CG1	2.96	0.41
1:A:313:LEU:O	1:A:317:CYS:HB2	2.21	0.41
1:C:80:ALA:HA	1:C:81:GLY:HA2	1.78	0.41
2:D:353:ILE:HD11	2:D:359:GLU:CB	2.48	0.41
2:B:273:VAL:H	1:C:376:ASN:ND2	2.09	0.41
2:D:32:GLY:HA2	2:D:94:THR:CG2	2.50	0.41

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	414/436 (95%)	398 (96%)	14 (3%)	2 (0%)	34	55
1	C	413/436 (95%)	401 (97%)	11 (3%)	1 (0%)	52	75
2	B	419/525 (80%)	406 (97%)	12 (3%)	1 (0%)	52	75
2	D	419/525 (80%)	406 (97%)	13 (3%)	0	100	100
All	All	1665/1922 (87%)	1611 (97%)	50 (3%)	4 (0%)	52	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	82	LEU
1	A	198	PRO
1	A	150	PHE
2	B	187	ASN

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	330/336 (98%)	290 (88%)	40 (12%)	6 11
1	C	330/336 (98%)	295 (89%)	35 (11%)	8 16
2	B	339/401 (84%)	307 (91%)	32 (9%)	11 20
2	D	339/401 (84%)	308 (91%)	31 (9%)	12 22
All	All	1338/1474 (91%)	1200 (90%)	138 (10%)	9 17

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	21	GLN
1	A	71	THR
1	A	74	LEU
1	A	87	LYS
1	A	104	ARG
1	A	121	LEU
1	A	122	ASP
1	A	123	ARG
1	A	128	LEU
1	A	129	SER
1	A	136	VAL
1	A	138	VAL
1	A	148	THR
1	A	164	THR
1	A	169	GLU
1	A	173	LEU
1	A	181	ASP
1	A	199	VAL
1	A	200	ARG
1	A	213	VAL
1	A	228	GLU
1	A	254	LEU
1	A	256	LEU

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Mol	Chain	Res	Type
1	A	269	LYS
1	A	274	THR
1	A	280	ARG
1	A	282	LYS
1	A	291	THR
1	A	292	LEU
1	A	306	GLU
1	A	320	LYS
1	A	329	LEU
1	A	343	SER
1	A	372	LEU
1	A	374	LEU
1	A	378	LEU
1	A	404	ASP
1	A	408	LEU
1	A	418	LEU
2	B	3	LEU
2	B	18	ARG
2	B	42	LEU
2	B	45	MSE
2	B	61	GLU
2	B	94	THR
2	B	100	LEU
2	B	101	GLN
2	B	108	SER
2	B	111	LEU
2	B	113	LEU
2	B	140	LEU
2	B	142	ARG
2	B	168	HIS
2	B	177	LYS
2	B	186	VAL
2	B	188	VAL
2	B	210	LEU
2	B	251	LYS
2	B	257	VAL
2	B	263	THR
2	B	264	LEU
2	B	266	GLN
2	B	269	TRP
2	B	274	ASP
2	B	308	VAL

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Mol	Chain	Res	Type
2	B	319	ARG
2	B	330	LEU
2	B	333	LEU
2	B	360	ARG
2	B	385	ARG
2	B	418	PHE
1	C	15	VAL
1	C	21	GLN
1	C	28	LEU
1	C	71	THR
1	C	73	VAL
1	C	74	LEU
1	C	76	GLU
1	C	77	GLN
1	C	82	LEU
1	C	97	LEU
1	C	98	GLU
1	C	100	ARG
1	C	118	LYS
1	C	119	LEU
1	C	121	LEU
1	C	128	LEU
1	C	138	VAL
1	C	148	THR
1	C	164	THR
1	C	173	LEU
1	C	188	LEU
1	C	199	VAL
1	C	201	MSE
1	C	213	VAL
1	C	239	LYS
1	C	254	LEU
1	C	274	THR
1	C	292	LEU
1	C	329	LEU
1	C	361	GLU
1	C	372	LEU
1	C	374	LEU
1	C	378	LEU
1	C	408	LEU
1	C	414	ARG
2	D	18	ARG

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Mol	Chain	Res	Type
2	D	41	LEU
2	D	45	MSE
2	D	61	GLU
2	D	100	LEU
2	D	111	LEU
2	D	113	LEU
2	D	140	LEU
2	D	142	ARG
2	D	150	ARG
2	D	159	LEU
2	D	168	HIS
2	D	188	VAL
2	D	210	LEU
2	D	218	SER
2	D	228	LYS
2	D	251	LYS
2	D	264	LEU
2	D	266	GLN
2	D	274	ASP
2	D	308	VAL
2	D	333	LEU
2	D	353	ILE
2	D	357	GLN
2	D	360	ARG
2	D	377	VAL
2	D	378	HIS
2	D	380	GLN
2	D	385	ARG
2	D	407	VAL
2	D	419	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	HIS
1	A	152	GLN
1	A	360	HIS
1	A	376	ASN
2	B	105	ASN
2	B	157	ASN
2	B	168	HIS
2	B	187	ASN

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Mol	Chain	Res	Type
2	B	204	GLN
2	B	229	GLN
2	B	266	GLN
2	B	380	GLN
1	C	77	GLN
1	C	132	HIS
1	C	135	HIS
1	C	152	GLN
1	C	216	ASN
1	C	360	HIS
1	C	376	ASN
2	D	13	HIS
2	D	31	HIS
2	D	105	ASN
2	D	157	ASN
2	D	168	HIS
2	D	204	GLN
2	D	206	HIS
2	D	229	GLN
2	D	266	GLN
2	D	378	HIS
2	D	380	GLN

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

2 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	$\#\|Z\| > 2$
3	SF4	A	425	1,2	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	C	425	1,2	0,12,12	0.00	-	0,24,24	0.00	-

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
3	SF4	A	425	1,2	-	0/0/48/48	0/6/5/5
3	SF4	C	425	1,2	-	0/0/48/48	0/6/5/5

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	425	SF4	1	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, 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	408/436 (93%)	-0.14	11 (2%) 58 62	26, 38, 51, 59	0
1	C	407/436 (93%)	-0.16	5 (1%) 81 83	23, 37, 51, 57	0
2	B	405/525 (77%)	-0.25	4 (0%) 84 86	25, 34, 46, 66	0
2	D	406/525 (77%)	-0.19	4 (0%) 84 86	27, 36, 47, 70	0
All	All	1626/1922 (84%)	-0.19	24 (1%) 76 79	23, 36, 50, 70	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	33[A]	TRP	5.4
2	D	421	ASP	5.0
1	A	82	LEU	4.2
1	C	7	THR	4.1
1	A	33[A]	TRP	3.5
1	C	134	PRO	3.1
1	A	7	THR	2.9
1	C	8	PHE	2.9
1	A	197	GLY	2.8
1	A	8	PHE	2.7
1	A	102	ASP	2.7
2	B	257	VAL	2.7
2	B	153	GLU	2.6
2	B	420	GLU	2.2
1	A	133	ALA	2.2
1	A	130	GLY	2.2
2	D	152	PRO	2.2
1	A	421	GLY	2.1
1	C	133	ALA	2.1
2	D	149	GLU	2.1
2	D	153	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	134	PRO	2.1
1	A	131	LEU	2.1
2	B	419	ARG	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 (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. 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
3	SF4	A	425	8/8	0.99	0.04	-2.96	23,25,26,26	0
3	SF4	C	425	8/8	0.99	0.04	-3.33	23,25,26,27	0

6.5 Other polymers (i)

There are no such residues in this entry.