Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2023 – 01:26 AM EDT

PDB ID	:	3AEK
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	:	2.30 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 (i) 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 (i)) were used in the production of this report:

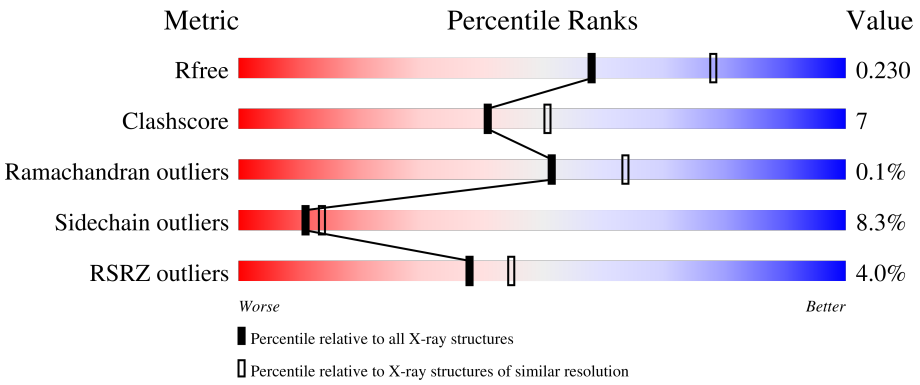
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	437	5%, 80%, 13%, • 5%
1	C	437	5%, 77%, 15%, • 5%
2	B	525	2%, 66%, 12%, • 20%
2	D	525	3%, 66%, 11%, • 20%

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	PMR	B	526	X	-	-	-
4	PMR	D	526	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13582 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	415	3164	2007	558	584	15	0	0	0
1	C	414	3169	2010	558	586	15	0	1	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	expression tag	UNP P26164
A	-11	ALA	-	expression tag	UNP P26164
A	-10	SER	-	expression tag	UNP P26164
A	-9	TRP	-	expression tag	UNP P26164
A	-8	SER	-	expression tag	UNP P26164
A	-7	HIS	-	expression tag	UNP P26164
A	-6	ALA	-	expression tag	UNP P26164
A	-5	PRO	-	expression tag	UNP P26164
A	-4	LYS	-	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	ALA	-	expression tag	UNP P26164
A	1	GLY	-	expression tag	UNP P26164
C	-12	MET	-	expression tag	UNP P26164
C	-11	ALA	-	expression tag	UNP P26164
C	-10	SER	-	expression tag	UNP P26164
C	-9	TRP	-	expression tag	UNP P26164
C	-8	SER	-	expression tag	UNP P26164
C	-7	HIS	-	expression tag	UNP P26164
C	-6	ALA	-	expression tag	UNP P26164
C	-5	PRO	-	expression tag	UNP P26164
C	-4	LYS	-	expression tag	UNP P26164
C	-3	PHE	-	expression tag	UNP P26164
C	-2	GLU	-	expression tag	UNP P26164

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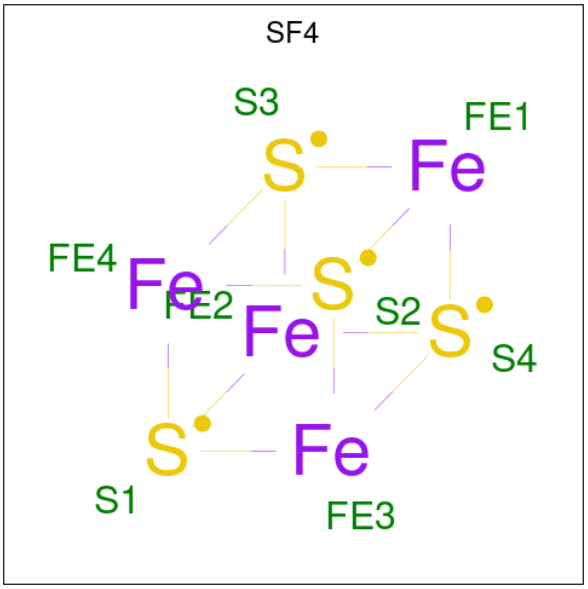
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	LYS	-	expression tag	UNP P26164
C	0	ALA	-	expression tag	UNP P26164
C	1	GLY	-	expression tag	UNP P26164

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

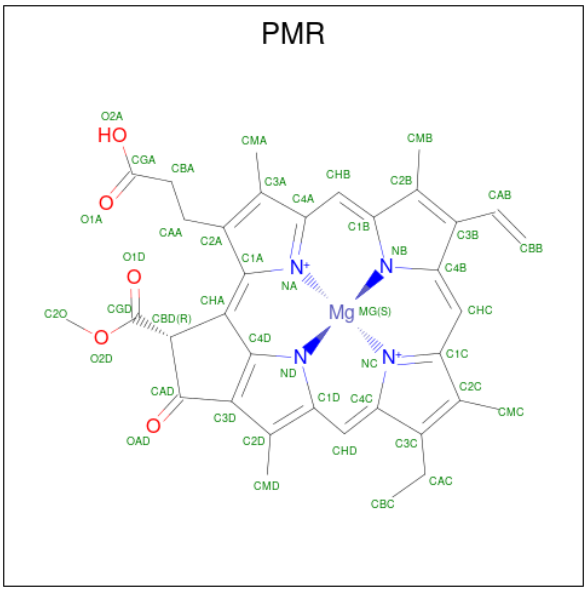
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	418	3209	2043	553	592	21	0	1	0
			Total	C	N	O	S			
2	D	418	3221	2050	559	591	21	0	2	0

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



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

- Molecule 4 is Protochlorophyllide (three-letter code: PMR) (formula: $C_{35}H_{32}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
4	B	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
4	D	1	45	35	1	4	5	0	0

- Molecule 5 is water.

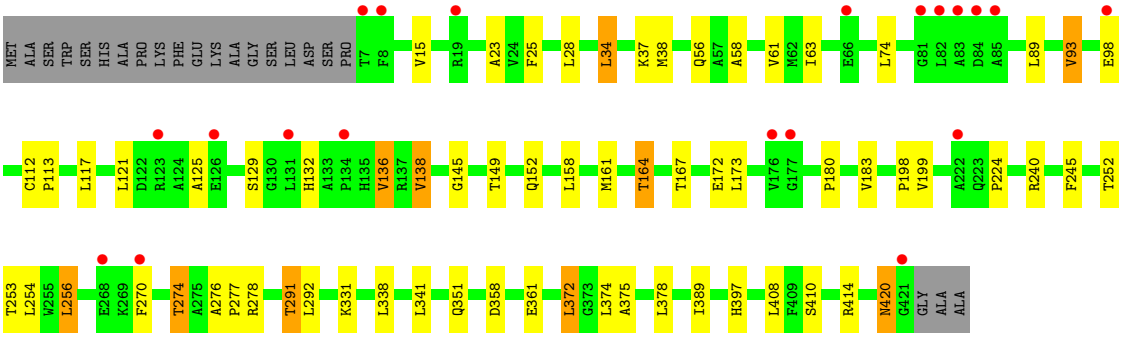
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	158	158	158	0	0
			Total	O		
5	B	199	199	199	0	0
			Total	O		
5	C	140	140	140	0	0
			Total	O		
5	D	216	216	216	0	0

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.

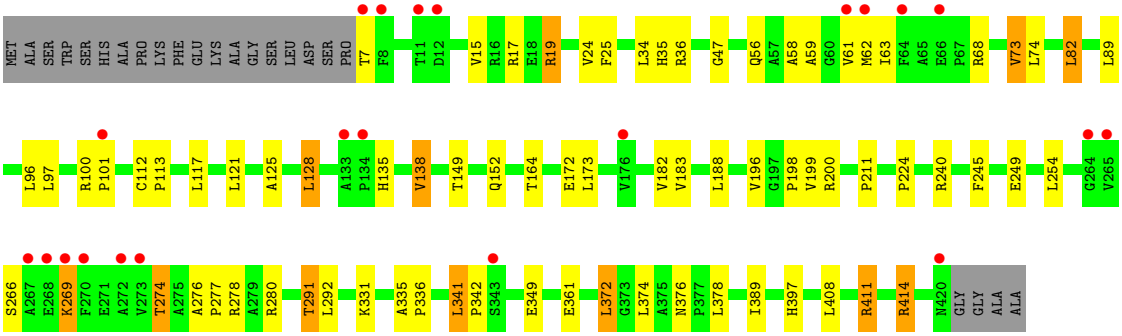
• Molecule 1: Light-independent protochlorophyllide reductase subunit N

Chain A:



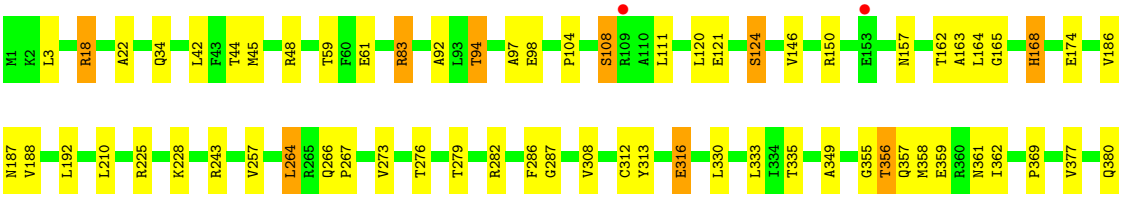
• Molecule 1: Light-independent protochlorophyllide reductase subunit N

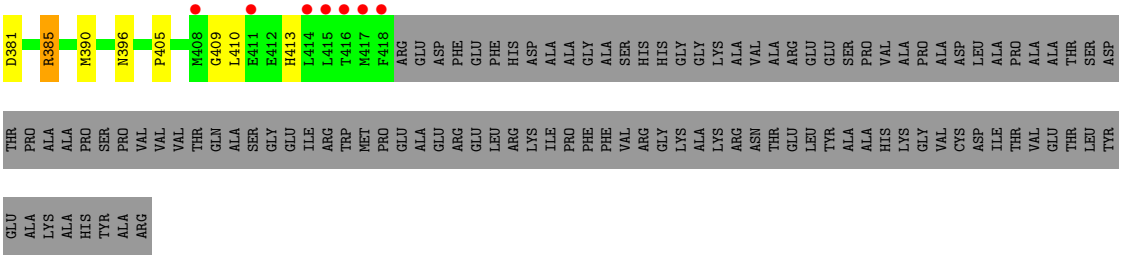
Chain C:



• Molecule 2: Light-independent protochlorophyllide reductase subunit B

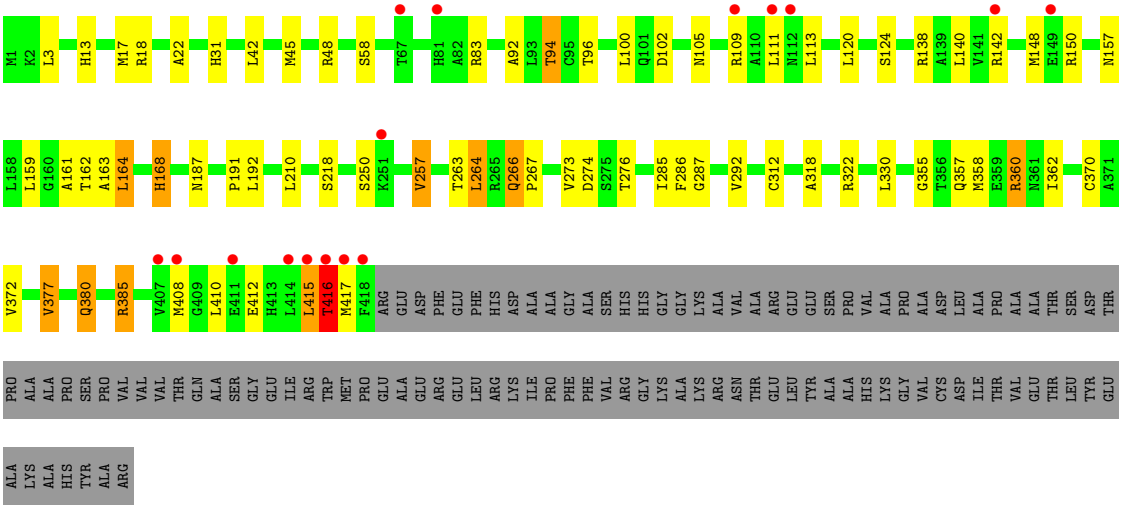
Chain B:





- 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	81.60Å 81.22Å 175.93Å 90.00° 100.86° 90.00°	Depositor
Resolution (Å)	34.06 – 2.30 34.05 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.06-2.30) 99.8 (34.05-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.191 , 0.232 0.191 , 0.230	Depositor DCC
R_{free} test set	5015 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	36.0	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13582	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 10.70% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, PMR

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	0.44	0/3227	0.60	0/4382
1	C	0.44	0/3232	0.61	0/4389
2	B	0.47	1/3280 (0.0%)	0.64	2/4465 (0.0%)
2	D	0.49	2/3293 (0.1%)	0.64	2/4481 (0.0%)
All	All	0.46	3/13032 (0.0%)	0.62	4/17717 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	148	MET	C-N	8.77	1.54	1.34
2	B	150	ARG	CZ-NH1	5.78	1.40	1.33
2	D	148	MET	C-O	5.65	1.34	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	150	ARG	NE-CZ-NH2	-7.41	116.60	120.30
2	D	150	ARG	NE-CZ-NH2	-5.62	117.49	120.30
2	D	415	LEU	C-N-CA	5.24	134.81	121.70
2	B	18	ARG	NE-CZ-NH2	-5.16	117.72	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3164	0	3199	41	0
1	C	3169	0	3201	40	0
2	B	3209	0	3231	49	0
2	D	3221	0	3250	53	0
3	A	8	0	0	0	0
3	C	8	0	0	0	0
4	B	45	0	31	6	0
4	D	45	0	31	12	0
5	A	158	0	0	4	0
5	B	199	0	0	3	0
5	C	140	0	0	5	0
5	D	216	0	0	1	0
All	All	13582	0	12943	183	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 7.

All (183) 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:D:380:GLN:HE21	2:D:380:GLN:H	1.12	0.97
1:A:164:THR:HB	5:A:531:HOH:O	1.71	0.90
2:B:273:VAL:H	1:C:376:ASN:HD21	1.20	0.89
2:B:162:THR:H	2:B:168:HIS:HD2	1.18	0.88
2:D:162:THR:H	2:D:168:HIS:HD2	1.18	0.86
2:B:356:THR:HG22	2:B:358:MET:H	1.40	0.84
4:D:526:PMR:HMC	4:D:526:PMR:HBCB	1.57	0.84
2:B:358:MET:HE3	2:B:362:ILE:HG13	1.61	0.83
1:A:149:THR:H	1:A:152:GLN:HE21	1.27	0.82
4:B:526:PMR:HBCB	4:B:526:PMR:HMC	1.59	0.82
1:A:34:LEU:HG	1:A:38:MET:CE	2.10	0.81
2:B:356:THR:HB	2:B:359:GLU:OE2	1.79	0.80
2:B:377:VAL:HG13	2:B:381:ASP:HB2	1.65	0.77
1:A:372:LEU:HD22	1:A:389:ILE:HD12	1.66	0.77
1:C:19:ARG:HH11	1:C:19:ARG:CG	2.00	0.74
1:A:420:ASN:C	1:A:420:ASN:HD22	1.91	0.74
1:C:149:THR:H	1:C:152:GLN:HE21	1.36	0.74
2:D:138:ARG:HD2	2:D:218:SER:HB3	1.71	0.73
2:B:157:ASN:HD21	2:B:187:ASN:HD22	1.37	0.72
2:D:157:ASN:HD21	2:D:187:ASN:HD22	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:358:MET:CE	2:B:362:ILE:HG13	2.20	0.71
2:D:380:GLN:H	2:D:380:GLN:NE2	1.88	0.71
4:B:526:PMR:HMC	4:B:526:PMR:CBC	2.21	0.71
4:D:526:PMR:HMC	4:D:526:PMR:CBC	2.23	0.69
1:C:291:THR:HG21	1:C:414:ARG:HD3	1.77	0.66
1:A:270:PHE:O	1:A:274:THR:HB	1.94	0.66
2:D:13:HIS:O	2:D:17:MET:HG3	1.96	0.65
2:B:276:THR:HG21	5:C:555:HOH:O	1.96	0.64
1:A:240:ARG:NH1	5:A:441:HOH:O	2.29	0.64
5:A:476:HOH:O	2:D:276:THR:HG21	1.98	0.64
1:C:19:ARG:HH11	1:C:19:ARG:HG3	1.62	0.64
2:D:31:HIS:HD2	2:D:58:SER:OG	1.82	0.62
4:B:526:PMR:HMCA	1:C:58:ALA:CB	2.29	0.62
4:B:526:PMR:HMCA	1:C:58:ALA:HB2	1.82	0.62
2:B:356:THR:HG22	2:B:358:MET:N	2.13	0.62
2:D:13:HIS:HD2	2:D:17:MET:CE	2.14	0.61
1:A:34:LEU:HG	1:A:38:MET:HE3	1.81	0.61
1:C:17:ARG:NH1	1:C:349:GLU:OE1	2.34	0.61
1:A:56:GLN:HA	1:A:63:ILE:HD13	1.83	0.60
5:C:535:HOH:O	2:D:45:MET:CE	2.50	0.59
1:A:291:THR:HG22	5:A:459:HOH:O	2.03	0.58
2:B:98:GLU:OE1	2:B:124:SER:HB2	2.04	0.58
4:D:526:PMR:HHC	4:D:526:PMR:HBB	1.86	0.57
2:B:157:ASN:HD22	2:B:188:VAL:H	1.53	0.57
1:C:101:PRO:O	1:C:135:HIS:HE1	1.88	0.57
1:A:23:ALA:H	1:A:351:GLN:NE2	2.03	0.56
1:A:58:ALA:CB	4:D:526:PMR:HMCA	2.35	0.56
2:D:286:PHE:O	2:D:355:GLY:HA2	2.04	0.56
2:B:377:VAL:CG1	2:B:381:ASP:HB2	2.34	0.56
2:D:161:ALA:O	2:D:191:PRO:HD2	2.06	0.56
1:A:410:SER:O	1:A:414:ARG:HG3	2.05	0.56
1:A:34:LEU:HG	1:A:38:MET:HE1	1.86	0.56
5:B:612:HOH:O	2:D:385:ARG:HD3	2.06	0.56
4:B:526:PMR:HMCB	1:C:25:PHE:CZ	2.41	0.55
1:C:240:ARG:NH2	5:C:533:HOH:O	2.39	0.55
5:C:535:HOH:O	2:D:45:MET:HE1	2.06	0.55
2:D:415:LEU:HB2	2:D:416:THR:OG1	2.07	0.55
1:C:372:LEU:HD22	1:C:389:ILE:HD12	1.88	0.55
2:B:225:ARG:O	2:B:228:LYS:HE3	2.07	0.54
1:A:58:ALA:HB2	4:D:526:PMR:HMCA	1.88	0.54
2:D:31:HIS:O	2:D:94:THR:HB	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:415:LEU:N	2:D:416:THR:HB	2.23	0.54
2:D:13:HIS:HD2	2:D:17:MET:HE2	1.74	0.52
1:C:17:ARG:HH22	1:C:331:LYS:HE2	1.74	0.52
4:B:526:PMR:HMAA	2:D:45:MET:HB3	1.92	0.52
1:C:128:LEU:HB3	1:C:138:VAL:HG11	1.91	0.52
1:A:158:LEU:HA	1:A:161:MET:HE3	1.92	0.51
2:B:44:THR:O	2:B:48:ARG:HA	2.10	0.51
2:D:18:ARG:HD2	2:D:163:ALA:O	2.10	0.51
1:A:253:THR:OG1	1:A:278:ARG:HD3	2.11	0.51
1:C:56:GLN:HA	1:C:63:ILE:HD13	1.93	0.51
1:C:274:THR:HG23	1:C:278:ARG:HE	1.76	0.50
2:D:358:MET:HE3	2:D:362:ILE:HG13	1.92	0.50
1:A:158:LEU:HD23	1:A:161:MET:CE	2.41	0.50
2:B:356:THR:CG2	2:B:358:MET:H	2.18	0.50
1:A:25:PHE:CZ	4:D:526:PMR:HMCB	2.46	0.50
1:C:82:LEU:HD11	1:C:117:LEU:O	2.12	0.50
2:B:286:PHE:O	2:B:355:GLY:HA2	2.12	0.50
1:C:36:ARG:HG3	1:C:62:MET:HE2	1.94	0.50
1:C:35:HIS:O	1:C:68:ARG:NH2	2.39	0.49
1:A:172:GLU:HG2	1:A:198:PRO:HD2	1.95	0.49
2:B:18:ARG:HD2	2:B:163:ALA:O	2.13	0.49
1:C:224:PRO:HA	1:C:245:PHE:CZ	2.48	0.48
1:A:23:ALA:H	1:A:351:GLN:HE22	1.59	0.48
2:D:105:ASN:O	2:D:109:ARG:HG3	2.13	0.48
2:D:372:VAL:HG11	2:D:377:VAL:CG2	2.44	0.48
2:D:22:ALA:HB1	2:D:192:LEU:HA	1.96	0.48
2:D:318:ALA:O	2:D:322:ARG:HG3	2.14	0.48
1:A:276:ALA:HB3	1:A:277:PRO:HD3	1.96	0.48
2:B:316:GLU:HG3	5:B:673:HOH:O	2.13	0.47
2:D:285:ILE:HG22	2:D:292:VAL:HG13	1.95	0.47
2:B:357:GLN:HE21	2:B:361:ASN:HD21	1.63	0.47
2:B:409:GLY:O	2:B:413:HIS:HD2	1.97	0.47
5:C:535:HOH:O	2:D:45:MET:HE3	2.13	0.47
2:B:162:THR:H	2:B:168:HIS:CD2	2.10	0.47
2:D:357:GLN:HE22	2:D:360[A]:ARG:CZ	2.28	0.47
1:C:372:LEU:HG	2:D:45:MET:SD	2.55	0.46
2:D:111:LEU:HB3	2:D:113:LEU:HD13	1.97	0.46
2:D:357:GLN:HE22	2:D:360[A]:ARG:NH1	2.12	0.46
2:D:358:MET:CE	2:D:362:ILE:HG13	2.44	0.46
2:B:273:VAL:H	1:C:376:ASN:ND2	2.01	0.46
1:C:249:GLU:OE2	1:C:278:ARG:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:THR:HG22	2:B:59:THR:O	2.15	0.46
2:D:157:ASN:ND2	2:D:187:ASN:HB3	2.30	0.46
4:D:526:PMR:HHC	4:D:526:PMR:CBB	2.45	0.46
2:B:396:ASN:HB3	2:D:385:ARG:HA	1.98	0.46
1:A:183:VAL:HG11	1:A:397:HIS:HB2	1.98	0.46
2:B:385:ARG:HD3	5:D:622:HOH:O	2.15	0.46
1:A:274:THR:CG2	1:A:278:ARG:HE	2.29	0.46
2:B:165:GLY:HA3	2:B:168:HIS:CD2	2.51	0.46
1:C:19:ARG:CG	1:C:19:ARG:NH1	2.67	0.45
2:B:243:ARG:NH1	5:B:595:HOH:O	2.49	0.45
2:B:45:MET:HB3	4:D:526:PMR:HMAA	1.98	0.45
1:A:224:PRO:HA	1:A:245:PHE:CZ	2.51	0.45
1:C:125:ALA:HA	1:C:138:VAL:HG22	1.97	0.45
2:D:31:HIS:HE1	2:D:102:ASP:OD1	1.99	0.45
1:C:335:ALA:HB3	1:C:336:PRO:HD3	1.97	0.45
2:D:18:ARG:HD3	2:D:164:LEU:HB3	1.98	0.44
1:A:112:CYS:HB2	1:A:113:PRO:HD3	1.97	0.44
2:D:13:HIS:CD2	2:D:17:MET:CE	2.97	0.44
2:B:316:GLU:H	2:B:316:GLU:HG2	1.32	0.44
2:B:22:ALA:HB1	2:B:192:LEU:HA	2.00	0.44
2:B:279:THR:HB	1:C:411:ARG:HD2	1.99	0.44
1:A:420:ASN:C	1:A:420:ASN:ND2	2.63	0.44
2:B:22:ALA:HB2	2:B:163:ALA:H	1.83	0.44
2:D:18:ARG:HD3	2:D:164:LEU:CB	2.47	0.44
1:A:125:ALA:HA	1:A:138:VAL:CG2	2.48	0.44
2:B:358:MET:CE	2:B:362:ILE:CG1	2.95	0.44
1:C:276:ALA:HB3	1:C:277:PRO:HD3	2.00	0.44
1:C:183:VAL:HG11	1:C:397:HIS:HB2	1.99	0.43
1:A:89:LEU:O	1:A:93:VAL:HG13	2.18	0.43
2:B:264:LEU:HD22	2:B:267:PRO:HD3	1.99	0.43
2:B:369:PRO:HB3	2:B:405:PRO:HB2	1.99	0.43
1:A:132:HIS:HB3	1:A:136:VAL:HG13	1.99	0.43
1:A:161:MET:O	1:A:164:THR:HG22	2.17	0.43
2:B:313:TYR:HA	2:B:335:THR:O	2.18	0.43
1:C:172:GLU:HG2	1:C:198:PRO:HD2	2.00	0.43
2:D:18:ARG:CD	2:D:163:ALA:O	2.67	0.43
2:D:264:LEU:HD22	2:D:267:PRO:HD3	2.00	0.43
2:B:385:ARG:NH1	2:D:385:ARG:HD2	2.33	0.43
2:D:266:GLN:HE21	2:D:267:PRO:N	2.17	0.43
4:D:526:PMR:HBB	4:D:526:PMR:CHC	2.48	0.43
2:D:250:SER:HB2	2:D:257:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:LEU:HD22	1:C:342:PRO:HD2	2.01	0.43
1:A:358:ASP:OD1	2:B:83:ARG:NH2	2.52	0.43
1:C:372:LEU:CD2	1:C:389:ILE:HD12	2.48	0.42
1:A:252:THR:HG22	1:A:256:LEU:HD22	2.01	0.42
2:D:92:ALA:HB2	2:D:120:LEU:HB2	1.99	0.42
1:C:59:ALA:O	1:C:62:MET:HB2	2.18	0.42
1:A:149:THR:N	1:A:152:GLN:HE21	2.06	0.42
1:A:375:ALA:HB1	2:D:273:VAL:HG21	2.02	0.42
2:B:356:THR:CG2	2:B:357:GLN:N	2.83	0.42
2:D:94:THR:HG22	2:D:96:THR:H	1.84	0.42
4:D:526:PMR:HBD	4:D:526:PMR:HAA	2.01	0.42
1:A:125:ALA:O	1:A:138:VAL:HG22	2.20	0.42
1:A:129:SER:HB3	1:A:138:VAL:H	1.85	0.41
2:B:380:GLN:H	2:B:380:GLN:CD	2.24	0.41
1:C:19:ARG:HH11	1:C:19:ARG:HG2	1.79	0.41
2:D:48:ARG:O	2:D:48:ARG:CG	2.68	0.41
2:D:360[A]:ARG:HG2	2:D:370:CYS:SG	2.60	0.41
2:B:282:ARG:NH2	2:B:308:VAL:HG21	2.35	0.41
1:C:200:ARG:HB2	1:C:211:PRO:HB3	2.02	0.41
2:D:380:GLN:HE21	2:D:380:GLN:N	1.94	0.41
4:D:526:PMR:HBD	4:D:526:PMR:O2A	2.20	0.41
2:B:92:ALA:HB2	2:B:120:LEU:HD12	2.01	0.41
1:C:266:SER:OG	1:C:269:LYS:HB2	2.20	0.41
1:A:338:LEU:HD23	1:A:341:LEU:HD12	2.02	0.41
4:D:526:PMR:HAA	4:D:526:PMR:CBD	2.50	0.41
1:A:180:PRO:HB3	2:D:417:MET:HB2	2.03	0.41
1:C:376:ASN:HD22	1:C:376:ASN:HA	1.68	0.41
2:B:174:GLU:HG2	2:B:390:MET:O	2.20	0.41
2:B:287:GLY:O	2:B:312:CYS:HA	2.20	0.41
1:C:47:GLY:O	1:C:73:VAL:HA	2.20	0.41
2:B:94:THR:HG22	2:B:97:ALA:H	1.86	0.41
2:B:104:PRO:O	2:B:108:SER:HB3	2.21	0.41
2:B:282:ARG:NH1	2:B:349:ALA:O	2.54	0.41
1:C:112:CYS:HB2	1:C:113:PRO:HD3	2.02	0.41
1:A:145:GLY:HA3	2:B:34:GLN:O	2.21	0.40
1:C:24:VAL:HB	1:C:149:THR:HG23	2.03	0.40
2:D:48:ARG:O	2:D:48:ARG:HG3	2.21	0.40
2:D:412:GLU:HA	2:D:415:LEU:HD13	2.03	0.40
1:A:113:PRO:O	1:A:117:LEU:HB2	2.21	0.40
2:D:287:GLY:O	2:D:312:CYS:HA	2.21	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	413/437 (94%)	404 (98%)	9 (2%)	0	100	100
1	C	413/437 (94%)	402 (97%)	11 (3%)	0	100	100
2	B	417/525 (79%)	413 (99%)	4 (1%)	0	100	100
2	D	418/525 (80%)	406 (97%)	11 (3%)	1 (0%)	47	58
All	All	1661/1924 (86%)	1625 (98%)	35 (2%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	416	THR

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	329/344 (96%)	302 (92%)	27 (8%)	11	14
1	C	330/344 (96%)	295 (89%)	35 (11%)	6	7
2	B	337/417 (81%)	314 (93%)	23 (7%)	16	21
2	D	338/417 (81%)	311 (92%)	27 (8%)	12	15
All	All	1334/1522 (88%)	1222 (92%)	112 (8%)	11	13

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	28	LEU
1	A	34	LEU
1	A	37	LYS
1	A	61	VAL
1	A	74	LEU
1	A	93	VAL
1	A	98	GLU
1	A	121	LEU
1	A	136	VAL
1	A	138	VAL
1	A	164	THR
1	A	167	THR
1	A	173	LEU
1	A	199	VAL
1	A	254	LEU
1	A	256	LEU
1	A	274	THR
1	A	291	THR
1	A	292	LEU
1	A	331	LYS
1	A	361	GLU
1	A	372	LEU
1	A	374	LEU
1	A	378	LEU
1	A	408	LEU
1	A	420	ASN
2	B	3	LEU
2	B	42	LEU
2	B	61	GLU
2	B	83	ARG
2	B	94	THR
2	B	108	SER
2	B	111	LEU
2	B	121	GLU
2	B	124	SER
2	B	146	VAL
2	B	164	LEU
2	B	168	HIS
2	B	186	VAL
2	B	210	LEU
2	B	257	VAL
2	B	264	LEU

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Mol	Chain	Res	Type
2	B	266	GLN
2	B	316	GLU
2	B	330	LEU
2	B	333	LEU
2	B	356	THR
2	B	385	ARG
2	B	410	LEU
1	C	7	THR
1	C	15	VAL
1	C	19	ARG
1	C	34	LEU
1	C	61	VAL
1	C	73	VAL
1	C	74	LEU
1	C	82	LEU
1	C	89	LEU
1	C	96	LEU
1	C	97	LEU
1	C	100	ARG
1	C	121	LEU
1	C	128	LEU
1	C	138	VAL
1	C	164	THR
1	C	173	LEU
1	C	182	VAL
1	C	188	LEU
1	C	196	VAL
1	C	199	VAL
1	C	254	LEU
1	C	269	LYS
1	C	274	THR
1	C	280	ARG
1	C	291	THR
1	C	292	LEU
1	C	341	LEU
1	C	361	GLU
1	C	372	LEU
1	C	374	LEU
1	C	378	LEU
1	C	408	LEU
1	C	411	ARG
1	C	414	ARG

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Mol	Chain	Res	Type
2	D	3	LEU
2	D	42	LEU
2	D	83	ARG
2	D	94	THR
2	D	100	LEU
2	D	124	SER
2	D	140	LEU
2	D	142[A]	ARG
2	D	142[B]	ARG
2	D	159	LEU
2	D	164	LEU
2	D	168	HIS
2	D	210	LEU
2	D	257	VAL
2	D	263	THR
2	D	264	LEU
2	D	266	GLN
2	D	274	ASP
2	D	330	LEU
2	D	360[A]	ARG
2	D	360[B]	ARG
2	D	377	VAL
2	D	380	GLN
2	D	385	ARG
2	D	408	MET
2	D	410	LEU
2	D	416	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	152	GLN
1	A	216	ASN
1	A	351	GLN
1	A	420	ASN
2	B	34	GLN
2	B	105	ASN
2	B	157	ASN
2	B	168	HIS
2	B	204	GLN
2	B	206	HIS

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Mol	Chain	Res	Type
2	B	229	GLN
2	B	266	GLN
2	B	361	ASN
2	B	413	HIS
1	C	35	HIS
1	C	39	GLN
1	C	135	HIS
1	C	152	GLN
1	C	216	ASN
1	C	376	ASN
2	D	31	HIS
2	D	34	GLN
2	D	64	HIS
2	D	105	ASN
2	D	157	ASN
2	D	168	HIS
2	D	204	GLN
2	D	222	HIS
2	D	229	GLN
2	D	266	GLN
2	D	357	GLN
2	D	361	ASN

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 monosaccharides 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	PMR	B	526	5	48,53,53	2.15	12 (25%)	54,89,89	1.61	7 (12%)
4	PMR	D	526	5	48,53,53	2.17	12 (25%)	54,89,89	1.47	7 (12%)
3	SF4	C	425	1,2	0,12,12	-	-	-		
3	SF4	A	425	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	PMR	B	526	5	3/3/16/20	5/15/111/111	-
3	SF4	C	425	1,2	-	-	0/6/5/5
4	PMR	D	526	5	3/3/16/20	5/15/111/111	-
3	SF4	A	425	1,2	-	-	0/6/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	526	PMR	MG-NB	-5.95	1.94	2.05
4	B	526	PMR	MG-NB	-5.79	1.94	2.05
4	D	526	PMR	C4D-CHA	-5.49	1.38	1.45
4	B	526	PMR	C4D-CHA	-5.05	1.38	1.45
4	B	526	PMR	MG-NC	-4.39	1.95	2.06
4	D	526	PMR	MG-NC	-4.35	1.95	2.06
4	D	526	PMR	MG-NA	-4.34	1.96	2.06
4	B	526	PMR	MG-NA	-4.16	1.96	2.06
4	D	526	PMR	C3D-CAD	-4.04	1.39	1.47
4	B	526	PMR	C3D-CAD	-3.94	1.39	1.47
4	D	526	PMR	C3B-C4B	-3.81	1.39	1.46
4	B	526	PMR	C3B-C4B	-3.71	1.39	1.46
4	B	526	PMR	C1B-C2B	-3.59	1.38	1.45
4	B	526	PMR	C4C-C3C	-3.14	1.39	1.45
4	B	526	PMR	C4A-C3A	-3.13	1.38	1.44
4	D	526	PMR	C1B-C2B	-3.12	1.39	1.45
4	D	526	PMR	C4C-C3C	-2.92	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	526	PMR	C4A-C3A	-2.83	1.39	1.44
4	D	526	PMR	C1C-C2C	-2.79	1.39	1.44
4	B	526	PMR	C1C-C2C	-2.75	1.39	1.44
4	B	526	PMR	CAB-C3B	-2.56	1.40	1.47
4	D	526	PMR	CAB-C3B	-2.48	1.40	1.47
4	B	526	PMR	C1A-C2A	-2.41	1.40	1.45
4	D	526	PMR	C1A-C2A	-2.40	1.40	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	526	PMR	C1A-NA-C4A	-6.85	103.63	106.71
4	B	526	PMR	O2D-CGD-CBD	5.06	120.26	111.27
4	D	526	PMR	C1A-NA-C4A	-5.01	104.45	106.71
4	D	526	PMR	O2D-CGD-CBD	4.51	119.29	111.27
4	D	526	PMR	C3C-C4C-NC	3.65	113.31	109.88
4	B	526	PMR	C3C-C4C-NC	3.35	113.03	109.88
4	D	526	PMR	O1D-CGD-CBD	-2.57	119.23	124.48
4	B	526	PMR	O1D-CGD-CBD	-2.54	119.28	124.48
4	B	526	PMR	CHC-C4B-NB	-2.25	122.38	124.45
4	B	526	PMR	CBD-CHA-C1A	2.16	132.91	128.88
4	B	526	PMR	O1A-CGA-CBA	-2.13	116.25	123.08
4	D	526	PMR	CBD-CHA-C1A	2.10	132.80	128.88
4	D	526	PMR	C4C-C3C-C2C	-2.08	103.86	106.90
4	D	526	PMR	O1A-CGA-CBA	-2.01	116.63	123.08

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	526	PMR	NA
4	B	526	PMR	NB
4	B	526	PMR	NC
4	D	526	PMR	NA
4	D	526	PMR	NB
4	D	526	PMR	NC

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	526	PMR	C2C-C3C-CAC-CBC
4	D	526	PMR	C2C-C3C-CAC-CBC
4	B	526	PMR	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
4	D	526	PMR	C4C-C3C-CAC-CBC
4	D	526	PMR	CAD-CBD-CGD-O2D
4	D	526	PMR	CAA-CBA-CGA-O1A
4	B	526	PMR	CAA-CBA-CGA-O1A
4	D	526	PMR	CAA-CBA-CGA-O2A
4	B	526	PMR	CAA-CBA-CGA-O2A
4	B	526	PMR	CAD-CBD-CGD-O2D

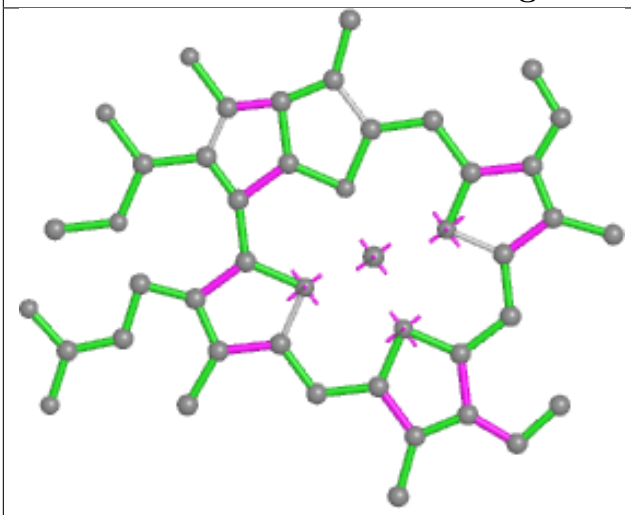
There are no ring outliers.

2 monomers are involved in 18 short contacts:

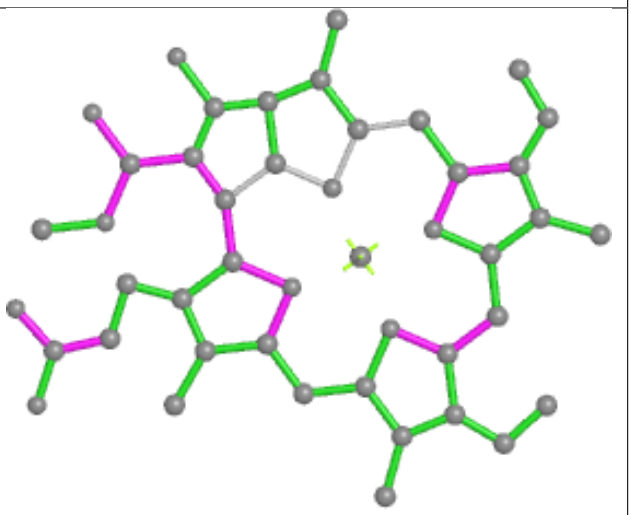
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	526	PMR	6	0
4	D	526	PMR	12	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

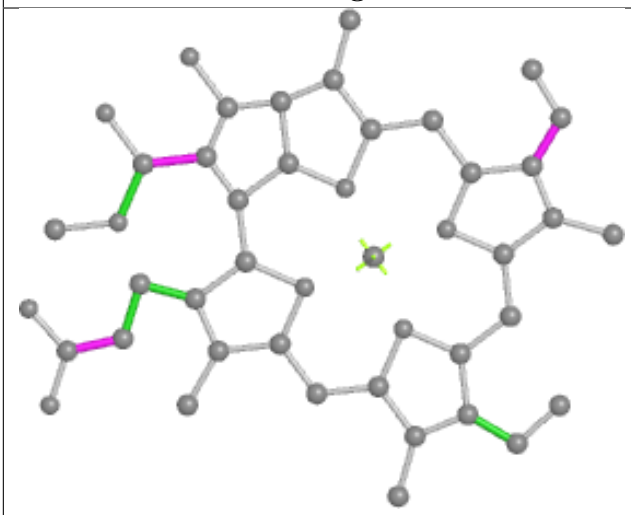
Ligand PMR B 526



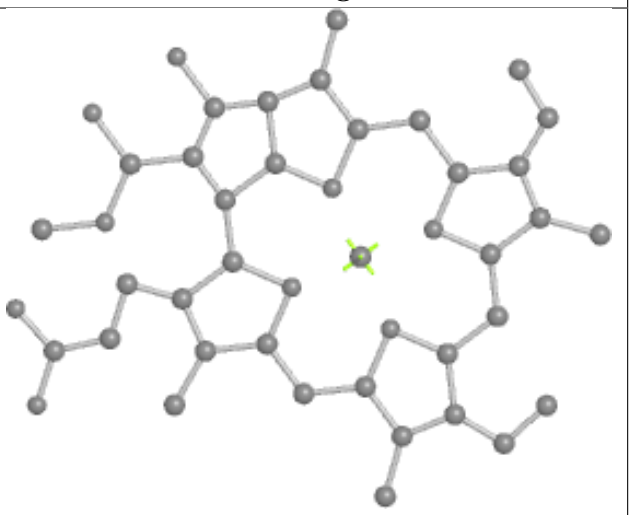
Bond lengths



Bond angles

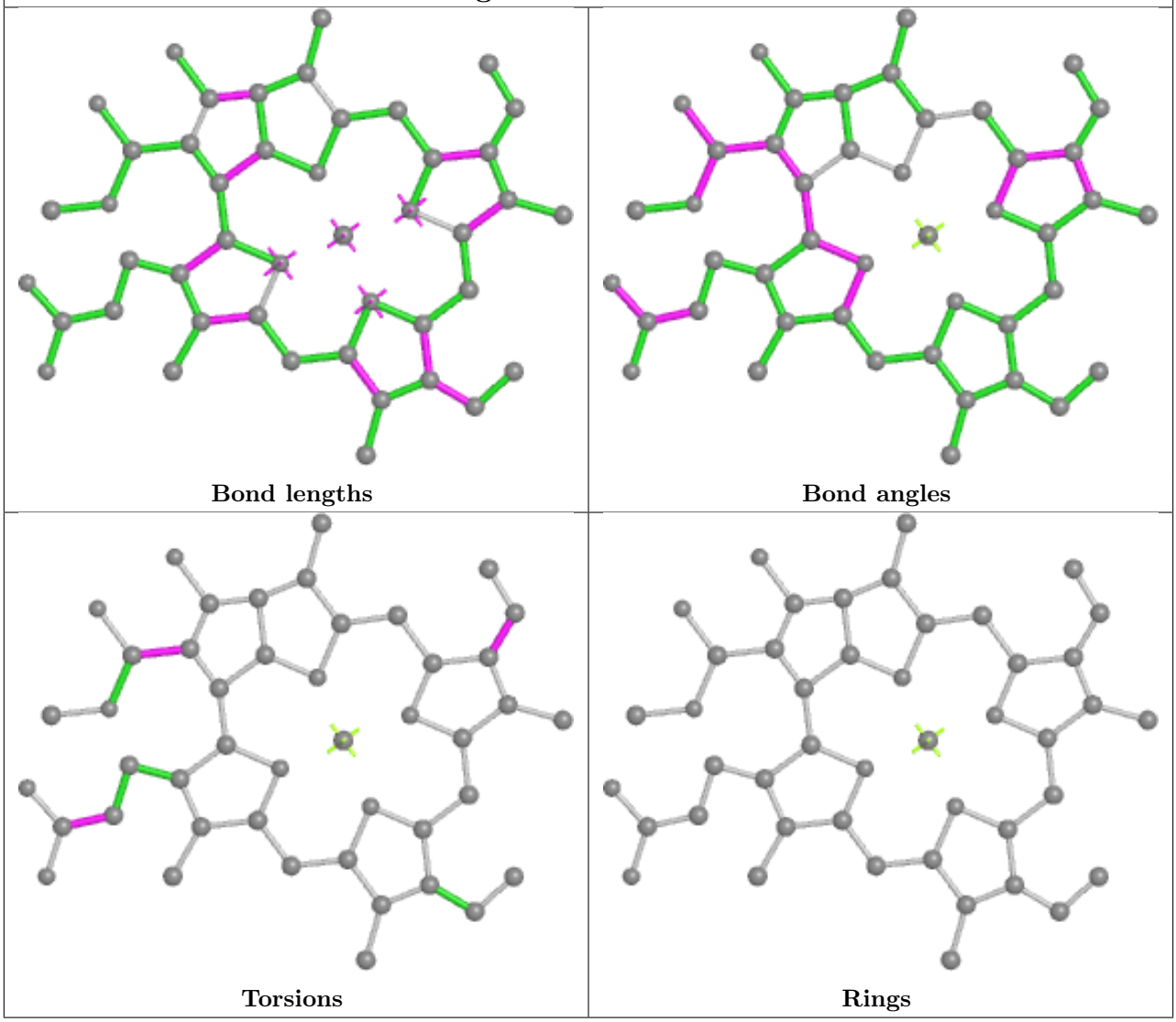


Torsions



Rings

Ligand PMR D 526



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	415/437 (94%)	0.35	20 (4%)	30	37	29, 36, 51, 59	0
1	C	414/437 (94%)	0.34	22 (5%)	26	33	29, 38, 49, 67	0
2	B	418/525 (79%)	0.08	9 (2%)	62	69	28, 34, 44, 75	0
2	D	418/525 (79%)	0.20	16 (3%)	40	47	28, 34, 42, 71	0
All	All	1665/1924 (86%)	0.24	67 (4%)	38	45	28, 36, 48, 75	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	415	LEU	8.7
2	B	418	PHE	7.7
1	A	83	ALA	6.6
2	B	415	LEU	6.3
1	C	7	THR	5.3
2	D	418	PHE	5.3
1	A	81	GLY	5.1
1	A	7	THR	4.6
2	D	416	THR	4.6
2	D	417	MET	4.3
1	C	8	PHE	4.2
1	A	8	PHE	4.2
2	B	416	THR	3.9
1	A	82	LEU	3.8
1	A	421	GLY	3.5
1	C	61	VAL	3.4
1	A	98	GLU	3.3
1	C	133	ALA	3.3
1	C	267	ALA	3.2
2	D	67	THR	3.1
1	A	131	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	126	GLU	3.0
1	A	176	VAL	2.9
2	D	408	MET	2.8
2	D	109	ARG	2.7
2	D	414	LEU	2.7
1	C	134	PRO	2.7
1	C	101	PRO	2.7
1	A	84	ASP	2.6
1	C	269	LYS	2.6
2	B	408	MET	2.6
1	C	176	VAL	2.6
1	C	62	MET	2.6
1	C	66	GLU	2.6
1	C	270	PHE	2.5
1	C	268	GLU	2.5
2	B	153	GLU	2.5
2	D	407	VAL	2.5
1	A	123	ARG	2.4
2	B	417	MET	2.4
1	C	343	SER	2.4
1	C	12	ASP	2.3
1	C	264	GLY	2.3
1	C	265	VAL	2.3
2	D	149	GLU	2.3
2	D	251	LYS	2.3
1	C	11	THR	2.2
1	A	66	GLU	2.2
2	D	81	HIS	2.2
2	D	112	ASN	2.2
1	A	19	ARG	2.2
2	B	414	LEU	2.2
1	A	270	PHE	2.2
2	B	109	ARG	2.1
1	A	268	GLU	2.1
2	B	411	GLU	2.1
1	C	272	ALA	2.1
1	C	64	PHE	2.1
1	C	420	ASN	2.1
2	D	142[A]	ARG	2.1
1	A	222	ALA	2.1
1	C	273	VAL	2.1
1	A	177	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	411	GLU	2.1
1	A	134	PRO	2.1
1	A	85	ALA	2.1
2	D	111	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

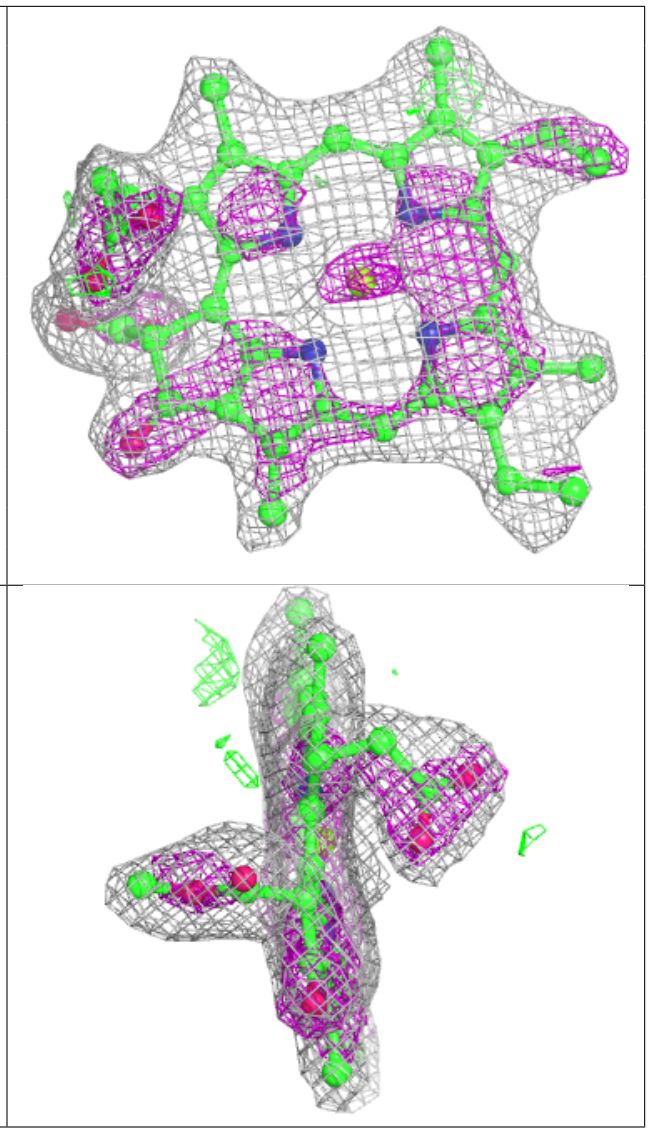
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PMR	B	526	45/45	0.95	0.16	34,36,38,42	0
4	PMR	D	526	45/45	0.95	0.17	33,35,36,36	0
3	SF4	A	425	8/8	0.99	0.03	25,25,26,27	0
3	SF4	C	425	8/8	0.99	0.03	25,26,27,30	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

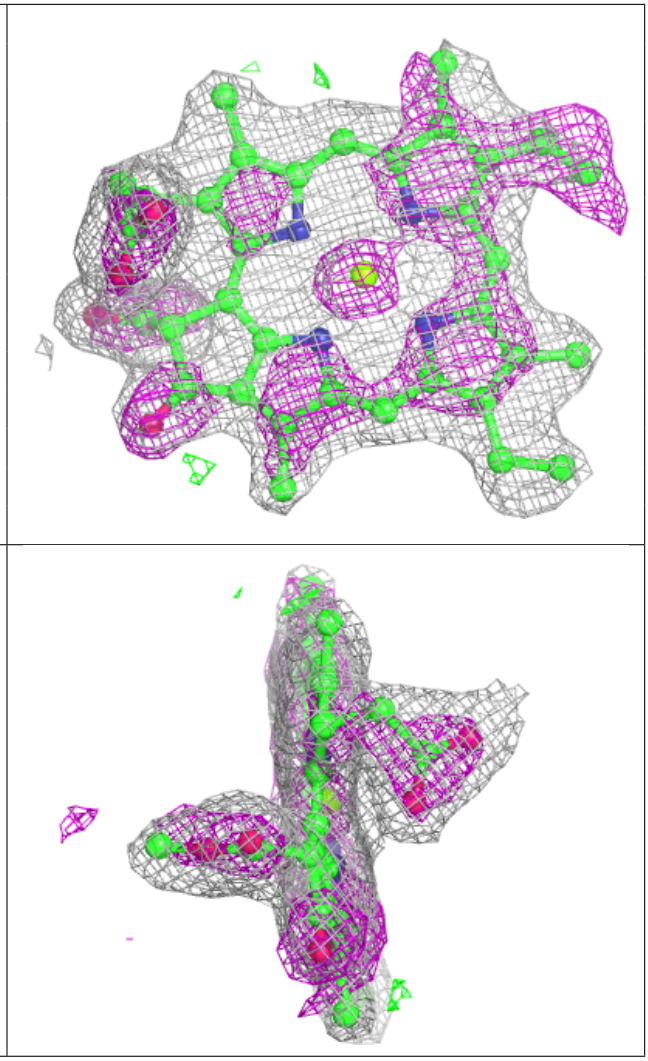
Electron density around PMR B 526:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PMR D 526:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.