



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:18 am BST

PDB ID : 3AEQ
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 : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

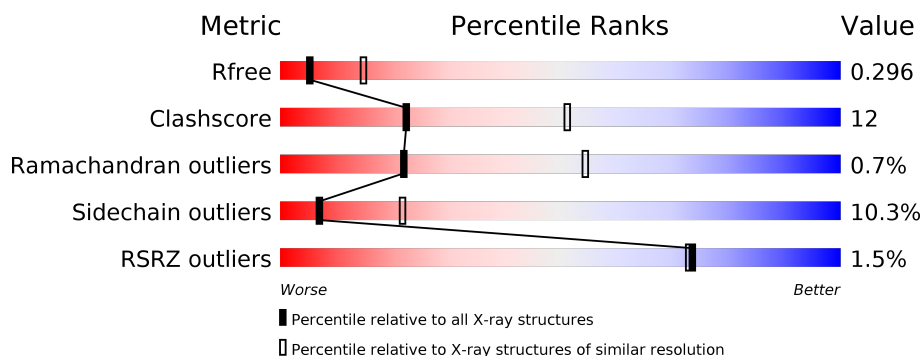
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	437	
1	C	437	
2	B	525	
2	D	525	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13035 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	0	0	0
			3164	2007	558	584	15			
1	C	414	Total	C	N	O	S	0	1	0
			3169	2010	558	586	15			

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	GLY	-	EXPRESSION TAG	UNP P26164
A	1	ALA	-	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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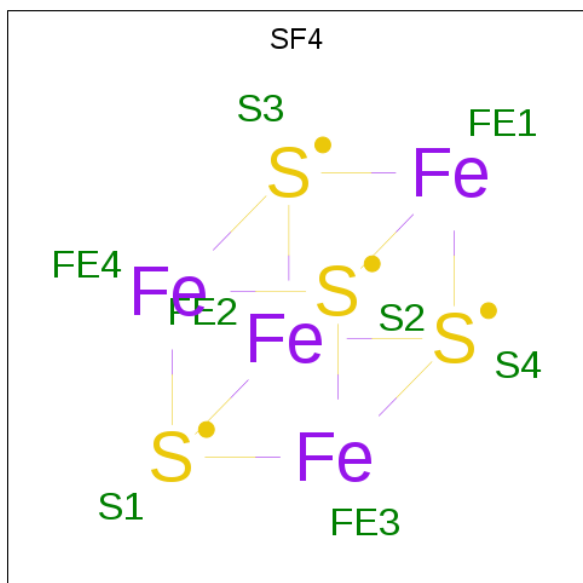
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	LYS	-	EXPRESSION TAG	UNP P26164
C	0	GLY	-	EXPRESSION TAG	UNP P26164
C	1	ALA	-	EXPRESSION TAG	UNP P26164

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

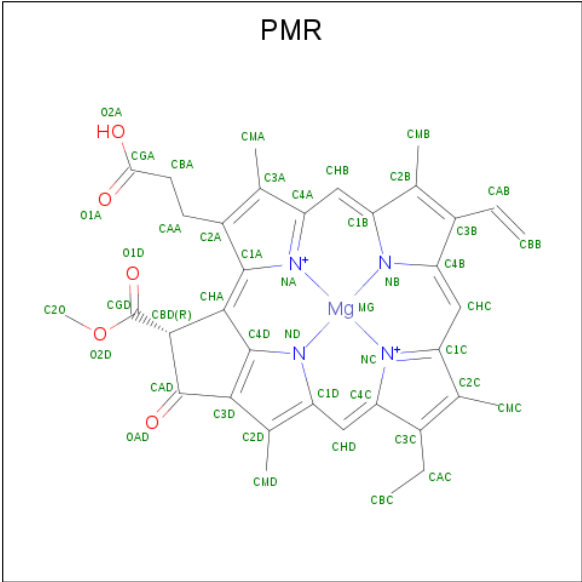
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	419	Total	C	N	O	S	0	16	0
			3297	2100	569	606	22			
2	D	419	Total	C	N	O	S	0	16	0
			3286	2092	568	604	22			

- 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 Protochlorophyllide (three-letter code: PMR) (formula: $\text{C}_{35}\text{H}_{32}\text{MgN}_4\text{O}_5$).



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

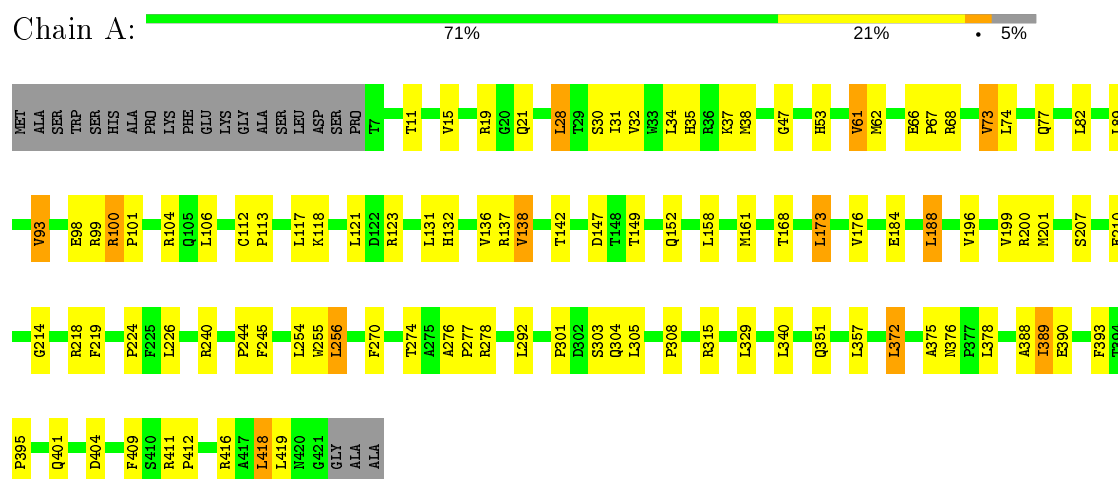
- Molecule 5 is water.

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

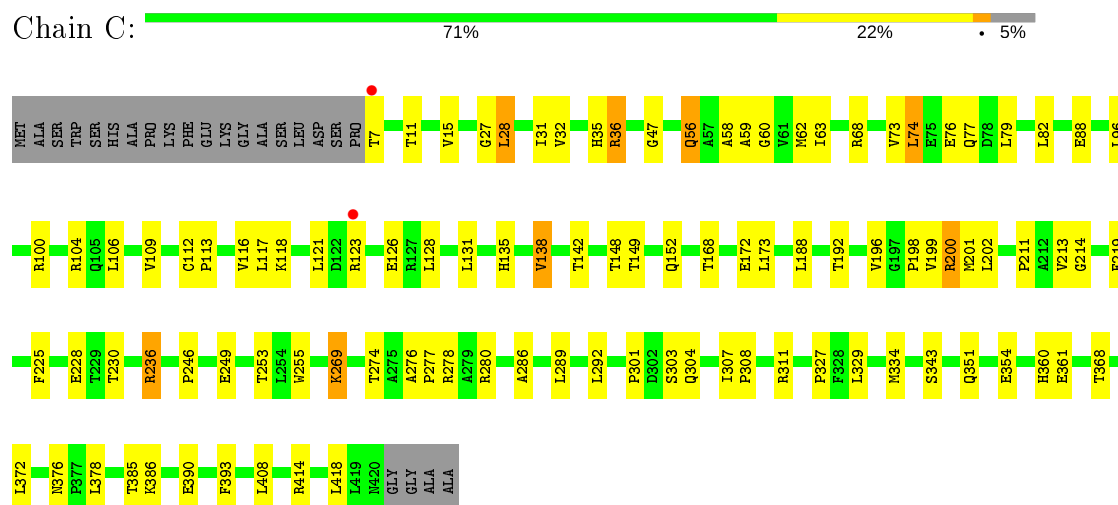
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Light-independent protochlorophyllide reductase subunit N

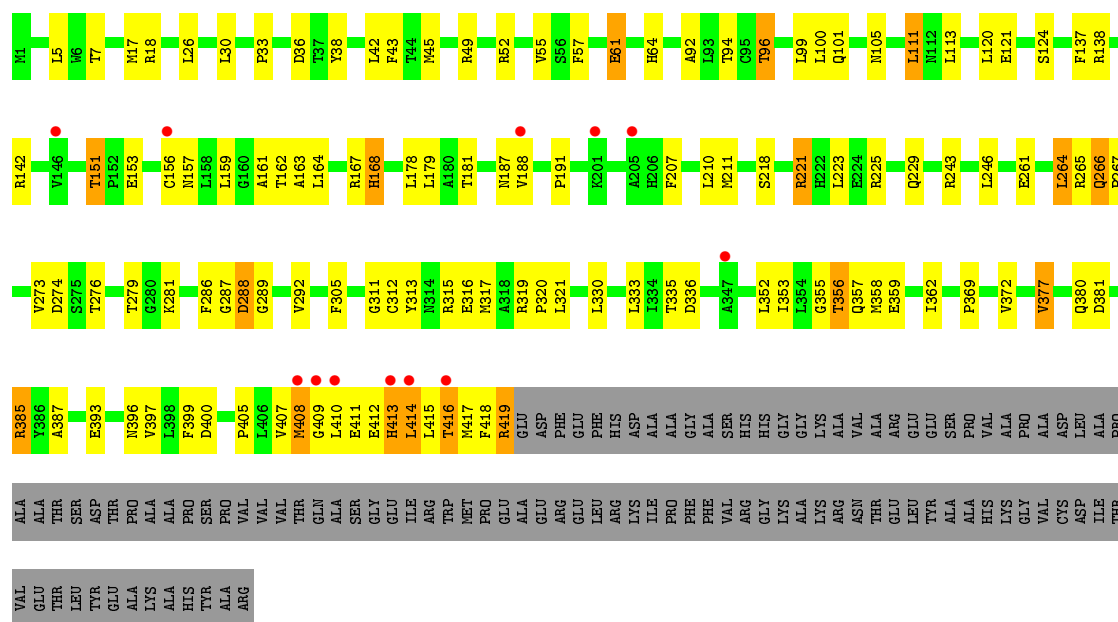


- Molecule 1: Light-independent protochlorophyllide reductase subunit N

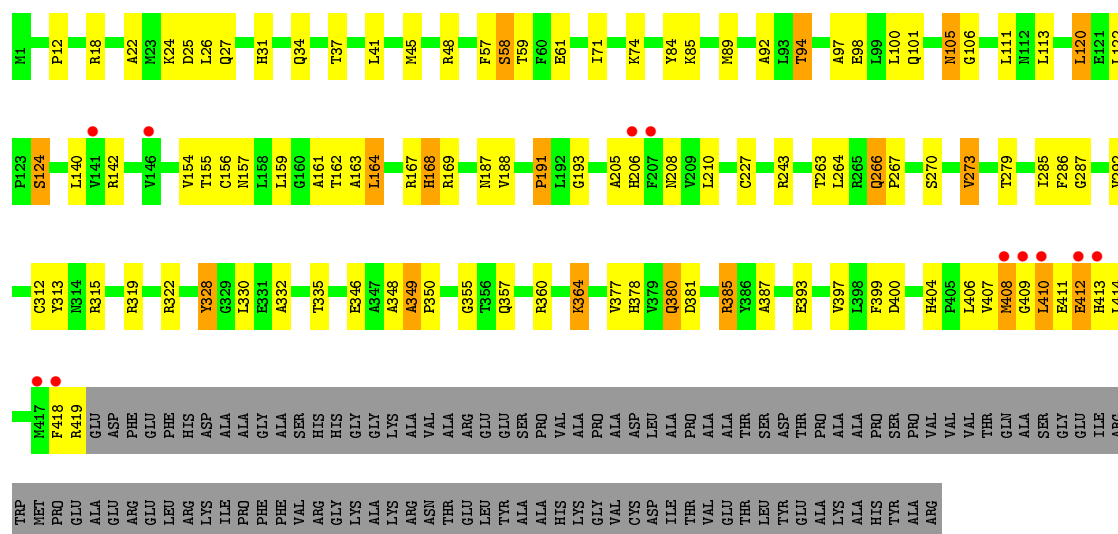


- Molecule 2: Light-independent protochlorophyllide reductase subunit B





• Molecule 2: Light-independent protochlorophyllide reductase subunit B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.63Å 81.28Å 177.10Å 90.00° 100.43° 90.00°	Depositor
Resolution (Å)	47.25 – 2.90 47.24 – 2.90	Depositor EDS
% Data completeness (in resolution range)	88.2 (47.25-2.90) 88.2 (47.24-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.235 , 0.298 0.236 , 0.296	Depositor DCC
R_{free} test set	2167 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	13035	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.47	0/3227	0.62	1/4382 (0.0%)
1	C	0.49	0/3232	0.64	1/4389 (0.0%)
2	B	0.50	0/3369	0.63	1/4581 (0.0%)
2	D	0.50	0/3357	0.64	0/4565
All	All	0.49	0/13185	0.63	3/17917 (0.0%)

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	D	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	418	LEU	CA-CB-CG	6.58	130.43	115.30
1	C	96	LEU	CA-CB-CG	6.22	129.61	115.30
2	B	264	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	410[A]	LEU	Peptide
2	D	412[A]	GLU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3164	0	3199	56	0
1	C	3169	0	3201	51	0
2	B	3297	0	3324	113	0
2	D	3286	0	3309	90	0
3	A	8	0	0	0	0
3	C	8	0	0	1	0
4	B	45	0	31	9	0
4	D	45	0	31	18	0
5	A	3	0	0	0	0
5	B	6	0	0	0	0
5	C	1	0	0	0	0
5	D	3	0	0	0	0
All	All	13035	0	13095	302	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 12.

All (302) 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:408[A]:MET:HB3	4:B:526:PMR:O2A	1.44	1.17
2:D:410[A]:LEU:O	2:D:413[A]:HIS:HB2	1.47	1.12
2:D:408[A]:MET:HG2	4:D:526:PMR:O1A	1.47	1.11
2:D:408[A]:MET:CG	4:D:526:PMR:CGA	2.29	1.09
2:B:414[B]:LEU:HA	2:B:417[B]:MET:CB	1.86	1.04
2:D:408[A]:MET:HG3	4:D:526:PMR:CGA	1.89	1.02
2:D:408[A]:MET:HG2	4:D:526:PMR:CGA	1.89	0.99
2:B:414[B]:LEU:HA	2:B:417[B]:MET:HB3	1.44	0.97
2:B:415[B]:LEU:O	2:B:419[B]:ARG:HD3	1.68	0.94
2:B:157:ASN:HD21	2:B:187:ASN:HD22	1.14	0.93
2:B:414[B]:LEU:CA	2:B:417[B]:MET:HB3	1.98	0.93
2:D:162:THR:H	2:D:168:HIS:HD2	1.15	0.93
2:B:414[B]:LEU:O	2:B:418[B]:PHE:CD2	2.23	0.92
4:D:526:PMR:HHC	4:D:526:PMR:HBB	1.56	0.88
2:B:410[A]:LEU:HD23	2:B:414[A]:LEU:HD23	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:THR:H	2:B:168:HIS:HD2	1.21	0.87
2:B:407[B]:VAL:HG23	2:B:408[B]:MET:CE	2.04	0.85
2:D:243:ARG:HH21	2:D:243:ARG:HG2	1.40	0.85
1:C:200:ARG:CG	1:C:200:ARG:HH11	1.89	0.84
2:B:414[B]:LEU:HA	2:B:417[B]:MET:HB2	1.57	0.84
2:B:412[B]:GLU:O	2:B:414[B]:LEU:N	2.11	0.83
1:C:149:THR:H	1:C:152:GLN:HE21	1.27	0.83
2:B:407[B]:VAL:HG23	2:B:408[B]:MET:HE2	1.61	0.82
2:B:408[A]:MET:CB	4:B:526:PMR:O2A	2.25	0.82
1:C:246:PRO:HD3	1:C:255:TRP:CD1	2.15	0.82
2:B:414[B]:LEU:HD22	2:B:417[B]:MET:HG2	1.60	0.81
2:D:74:LYS:HG3	2:D:111:LEU:HD11	1.62	0.81
2:B:413[B]:HIS:O	2:B:414[B]:LEU:HG	1.84	0.78
4:B:526:PMR:HMC	4:B:526:PMR:HBCB	1.66	0.78
2:B:157:ASN:HD21	2:B:187:ASN:ND2	1.83	0.76
2:B:414[B]:LEU:O	2:B:418[B]:PHE:CE2	2.37	0.76
1:A:188:LEU:HD13	1:A:201:MET:CE	2.15	0.76
2:B:409[A]:GLY:N	4:B:526:PMR:O2A	2.19	0.75
2:B:416[B]:THR:HA	2:B:419[B]:ARG:HB2	1.68	0.75
2:D:18:ARG:HD3	2:D:164:LEU:HB3	1.69	0.74
1:C:35:HIS:O	1:C:68:ARG:NH2	2.20	0.74
1:C:200:ARG:HG2	1:C:200:ARG:HH11	1.52	0.74
2:D:410[A]:LEU:HD12	4:D:526:PMR:C2D	2.18	0.74
1:A:34:LEU:HG	1:A:38:MET:HE1	1.69	0.73
1:C:386:LYS:NZ	1:C:390:GLU:OE1	2.21	0.73
2:B:412[B]:GLU:OE1	2:B:415[B]:LEU:HD12	1.89	0.72
2:B:151:THR:HB	2:B:153:GLU:O	1.88	0.72
2:B:356:THR:HG22	2:B:358:MET:H	1.55	0.72
2:B:413[B]:HIS:O	2:B:414[B]:LEU:HD23	1.90	0.72
2:B:264:LEU:HD11	2:B:267:PRO:HG2	1.71	0.71
1:A:112:CYS:HB3	2:B:96:THR:HG21	1.73	0.71
1:A:200:ARG:NH1	1:A:200:ARG:HB2	2.06	0.71
2:B:162:THR:H	2:B:168:HIS:CD2	2.06	0.71
1:C:56:GLN:HA	1:C:63:ILE:HD13	1.73	0.71
2:D:98:GLU:OE1	2:D:124:SER:HB2	1.92	0.70
2:D:31:HIS:O	2:D:94:THR:HB	1.92	0.69
1:C:276:ALA:HB3	1:C:277:PRO:HD3	1.73	0.68
2:B:413[B]:HIS:O	2:B:414[B]:LEU:CG	2.42	0.68
2:D:162:THR:H	2:D:168:HIS:CD2	2.05	0.68
2:B:418[B]:PHE:O	2:B:419[B]:ARG:C	2.30	0.68
2:B:407[B]:VAL:HG23	2:B:408[B]:MET:HE3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:THR:N	2:B:168:HIS:HD2	1.93	0.67
2:B:413[B]:HIS:O	2:B:414[B]:LEU:CD2	2.42	0.67
2:B:266:GLN:HE21	2:B:267:PRO:N	1.93	0.67
2:B:356:THR:HB	2:B:359:GLU:OE2	1.95	0.67
2:B:410[A]:LEU:CD2	2:B:414[A]:LEU:HD23	2.25	0.67
2:B:412[B]:GLU:C	2:B:414[B]:LEU:H	1.99	0.66
1:A:274:THR:CG2	1:A:278:ARG:HE	2.09	0.66
2:D:410[A]:LEU:HD12	4:D:526:PMR:C1D	2.26	0.66
2:D:380:GLN:H	2:D:380:GLN:HE21	1.44	0.65
1:A:276:ALA:HB3	1:A:277:PRO:HD3	1.79	0.64
2:B:167:ARG:HD2	2:B:387:ALA:O	1.98	0.64
2:D:410[A]:LEU:O	2:D:413[A]:HIS:CB	2.37	0.64
1:A:112:CYS:HB2	1:A:113:PRO:HD3	1.79	0.64
1:A:184:GLU:OE2	1:A:201:MET:HG3	1.97	0.63
2:B:414[B]:LEU:C	2:B:417[B]:MET:HB3	2.18	0.63
2:D:408[A]:MET:HG3	4:D:526:PMR:O2A	1.99	0.62
2:D:407[B]:VAL:O	2:D:411[B]:GLU:HB2	1.99	0.62
4:B:526:PMR:HMAA	2:D:45:MET:HB3	1.81	0.62
2:B:157:ASN:HD22	2:B:188:VAL:H	1.47	0.61
2:D:407[A]:VAL:O	2:D:408[A]:MET:O	2.18	0.61
2:B:36:ASP:OD2	2:B:94:THR:HG21	2.00	0.61
2:D:418[B]:PHE:O	2:D:419[B]:ARG:O	2.18	0.61
2:D:157:ASN:HD21	2:D:187:ASN:HD22	1.49	0.61
2:D:414[B]:LEU:O	2:D:418[B]:PHE:CD2	2.53	0.61
2:D:414[B]:LEU:HD22	2:D:418[B]:PHE:CE2	2.36	0.60
1:C:200:ARG:HH11	1:C:200:ARG:HG3	1.66	0.60
2:D:380:GLN:H	2:D:380:GLN:NE2	1.99	0.60
1:A:372:LEU:HD22	1:A:389:ILE:HD13	1.84	0.60
2:B:157:ASN:ND2	2:B:187:ASN:HD22	1.93	0.60
2:B:43:PHE:HB3	2:B:49:ARG:HD2	1.84	0.60
4:D:526:PMR:HBD	4:D:526:PMR:O2A	2.00	0.59
1:A:158:LEU:HA	1:A:161:MET:HE3	1.83	0.59
1:A:224:PRO:HA	1:A:245:PHE:CZ	2.37	0.59
1:A:34:LEU:HG	1:A:38:MET:CE	2.33	0.59
2:B:358:MET:HE3	2:B:362:ILE:HG13	1.84	0.59
2:D:18:ARG:HD2	2:D:163:ALA:O	2.02	0.58
1:C:253:THR:OG1	1:C:278:ARG:HD3	2.03	0.58
1:C:28:LEU:HD22	3:C:425:SF4:S2	2.43	0.58
1:A:274:THR:O	1:A:278:ARG:HB2	2.03	0.58
2:D:92:ALA:HB2	2:D:120:LEU:HD12	1.86	0.58
2:D:243:ARG:HH21	2:D:243:ARG:CG	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:286:PHE:O	2:B:355:GLY:HA2	2.04	0.57
2:B:45:MET:HB3	4:D:526:PMR:HMAA	1.86	0.57
2:B:407[B]:VAL:O	2:B:411[B]:GLU:HB2	2.05	0.57
2:D:243:ARG:NH2	2:D:243:ARG:HG2	2.17	0.57
2:D:407[B]:VAL:C	2:D:409[B]:GLY:H	2.09	0.57
1:A:106:LEU:HB3	1:A:138:VAL:HB	1.85	0.57
1:A:117:LEU:HD11	2:B:99:LEU:HD22	1.86	0.56
2:D:94:THR:HG22	2:D:97:ALA:H	1.70	0.56
1:A:132:HIS:HB3	1:A:136:VAL:HG13	1.88	0.56
1:A:32:VAL:HG12	1:A:393:PHE:HZ	1.70	0.56
2:B:7:THR:HG23	2:B:7:THR:O	2.04	0.56
2:D:418[B]:PHE:O	2:D:419[B]:ARG:C	2.44	0.55
2:D:287:GLY:O	2:D:312:CYS:HA	2.07	0.55
2:D:31:HIS:HA	2:D:58:SER:OG	2.07	0.55
2:B:356:THR:CG2	2:B:358:MET:H	2.20	0.55
1:C:225:PHE:HA	1:C:304:GLN:NE2	2.22	0.55
2:D:22:ALA:HB2	2:D:163:ALA:H	1.71	0.55
2:B:356:THR:HG23	2:B:357:GLN:N	2.22	0.55
2:B:30:LEU:HD12	2:B:57:PHE:CZ	2.42	0.55
2:D:48:ARG:O	2:D:48:ARG:HG3	2.06	0.54
2:B:407[B]:VAL:CG2	2:B:408[B]:MET:HE3	2.37	0.54
1:C:414:ARG:O	1:C:418:LEU:HB2	2.07	0.54
2:D:27:GLN:HB2	2:D:89:MET:HG2	1.89	0.54
2:B:161:ALA:HB2	2:B:211:MET:HE3	1.90	0.54
2:B:264:LEU:CD1	2:B:267:PRO:HG2	2.38	0.54
2:D:313:TYR:HA	2:D:335:THR:O	2.08	0.53
2:D:357:GLN:HE21	2:D:378:HIS:H	1.56	0.53
2:D:411[A]:GLU:O	2:D:412[A]:GLU:C	2.45	0.53
2:B:414[B]:LEU:O	2:B:418[B]:PHE:HD2	1.89	0.53
2:B:412[B]:GLU:OE1	2:B:415[B]:LEU:CD1	2.55	0.53
1:A:67:PRO:HD2	2:B:5:LEU:HD21	1.89	0.53
2:B:221:ARG:O	2:B:225:ARG:HG3	2.08	0.53
1:C:307:ILE:HB	1:C:334:MET:HE3	1.92	0.52
2:B:17:MET:HG2	2:B:55:VAL:HG21	1.92	0.52
2:B:393:GLU:O	2:B:397:VAL:HG23	2.10	0.52
4:B:526:PMR:HMCA	1:C:58:ALA:CB	2.39	0.52
2:B:178:LEU:HD13	2:B:246:LEU:HD21	1.92	0.52
4:B:526:PMR:HACA	1:C:393:PHE:CE2	2.45	0.52
2:B:414[B]:LEU:HD22	2:B:417[B]:MET:CG	2.36	0.51
2:D:348:ALA:O	2:D:350:PRO:HD3	2.10	0.51
1:A:207:SER:O	1:A:210:GLU:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:ASP:O	2:B:292:VAL:HG23	2.11	0.51
2:B:412[B]:GLU:HA	2:B:415[B]:LEU:HD12	1.91	0.51
2:D:322:ARG:HG2	2:D:332:ALA:HB3	1.92	0.51
2:D:41:LEU:O	2:D:45:MET:HB2	2.11	0.51
2:B:369:PRO:HB3	2:B:405[B]:PRO:HB2	1.92	0.51
2:D:167:ARG:HD2	2:D:387:ALA:O	2.11	0.51
2:B:92:ALA:HB2	2:B:120:LEU:HD12	1.93	0.50
2:D:111:LEU:HB3	2:D:113:LEU:CD1	2.41	0.50
2:D:286:PHE:O	2:D:355:GLY:HA2	2.11	0.50
4:D:526:PMR:CGD	4:D:526:PMR:HAA	2.41	0.50
1:C:112:CYS:HB2	1:C:113:PRO:HD3	1.94	0.50
1:A:372:LEU:HD22	1:A:389:ILE:CD1	2.41	0.50
1:C:123:ARG:O	1:C:126:GLU:HB3	2.12	0.50
2:D:409[A]:GLY:O	2:D:410[A]:LEU:O	2.30	0.50
2:B:418[B]:PHE:O	2:B:419[B]:ARG:O	2.30	0.49
1:C:59:ALA:HB1	1:C:62:MET:HB3	1.94	0.49
2:B:138:ARG:HD3	2:B:218:SER:HB3	1.94	0.49
2:B:413[B]:HIS:C	2:B:414[B]:LEU:HG	2.32	0.49
2:D:155:THR:H	2:D:206:HIS:HD2	1.58	0.49
2:D:243:ARG:NH2	2:D:243:ARG:CG	2.72	0.49
2:D:285:ILE:HG22	2:D:292:VAL:HG13	1.94	0.49
1:A:158:LEU:HA	1:A:161:MET:CE	2.43	0.49
1:C:149:THR:H	1:C:152:GLN:NE2	2.04	0.48
2:B:313:TYR:HA	2:B:335:THR:O	2.13	0.48
1:C:172:GLU:HG2	1:C:198:PRO:HG2	1.95	0.48
1:C:286:ALA:HA	1:C:289:LEU:HD12	1.96	0.48
2:B:7:THR:CG2	2:B:7:THR:O	2.60	0.48
1:A:30:SER:O	1:A:34:LEU:HB2	2.13	0.48
1:C:200:ARG:CG	1:C:200:ARG:NH1	2.59	0.48
2:B:273:VAL:H	1:C:376:ASN:HD21	1.60	0.48
1:C:354:GLU:OE1	1:C:354:GLU:HA	2.12	0.48
2:D:48:ARG:O	2:D:48:ARG:CG	2.62	0.48
2:D:408[A]:MET:CG	4:D:526:PMR:O1A	2.31	0.48
2:B:156:CYS:HB3	2:B:207:PHE:CE2	2.49	0.48
1:C:308:PRO:HD3	1:C:334:MET:HE3	1.95	0.48
1:A:61:VAL:HG23	2:D:410[A]:LEU:HD23	1.95	0.48
1:A:200:ARG:HB2	1:A:200:ARG:HH11	1.78	0.48
2:B:319:ARG:HB3	2:B:320:PRO:HD3	1.96	0.47
1:C:31:ILE:HD11	1:C:109:VAL:HG21	1.96	0.47
1:C:303:SER:O	1:C:304:GLN:HB2	2.14	0.47
4:B:526:PMR:HMCA	1:C:58:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:266:GLN:HE21	2:D:267:PRO:N	2.12	0.47
2:D:377:VAL:CG2	2:D:381:ASP:HB2	2.44	0.47
2:B:418[B]:PHE:HE1	1:C:36:ARG:HE	1.62	0.47
1:A:255:TRP:HE3	1:A:256:LEU:HD13	1.80	0.47
2:B:312:CYS:SG	2:B:321:LEU:HD22	2.54	0.47
1:A:188:LEU:HD13	1:A:201:MET:HE3	1.92	0.47
1:A:395:PRO:HB2	1:A:401:GLN:HG2	1.96	0.47
1:A:276:ALA:HB3	1:A:277:PRO:CD	2.44	0.47
2:B:377:VAL:CG1	2:B:381:ASP:HB2	2.44	0.47
2:D:157:ASN:HB2	2:D:208:ASN:OD1	2.15	0.47
4:B:526:PMR:CBC	4:B:526:PMR:HMC	2.40	0.46
2:B:377:VAL:HG13	2:B:381:ASP:HB2	1.97	0.46
2:B:38:TYR:C	2:B:38:TYR:CD2	2.87	0.46
2:D:270:SER:HB3	2:D:399:PHE:CE1	2.50	0.46
1:A:28:LEU:O	1:A:31:ILE:HD12	2.15	0.46
2:B:336:ASP:C	2:B:336:ASP:OD1	2.53	0.46
2:D:406[A]:LEU:O	2:D:407[A]:VAL:HG22	2.14	0.46
2:B:356:THR:CG2	2:B:357:GLN:N	2.77	0.46
2:B:408[B]:MET:O	2:B:412[B]:GLU:HG2	2.15	0.46
4:D:526:PMR:HMC	4:D:526:PMR:HBCB	1.96	0.46
1:A:219:PHE:CE2	1:A:240:ARG:HG3	2.51	0.46
1:A:315:ARG:HD2	1:A:340:LEU:O	2.16	0.46
2:B:18:ARG:HD2	2:B:163:ALA:O	2.16	0.46
2:B:223:LEU:HB3	2:B:229:GLN:HE21	1.80	0.46
2:D:84:TYR:O	2:D:85:LYS:C	2.53	0.46
1:A:99:ARG:O	1:A:101:PRO:HD3	2.16	0.46
1:A:68:ARG:HG2	1:A:100:ARG:NH1	2.31	0.45
1:A:376:ASN:OD1	2:D:273:VAL:HB	2.16	0.45
2:B:157:ASN:ND2	2:B:188:VAL:H	2.13	0.45
1:A:200:ARG:HB2	1:A:200:ARG:CZ	2.46	0.45
2:B:137:PHE:CD1	2:B:191:PRO:HG3	2.51	0.45
2:D:157:ASN:HD22	2:D:188:VAL:H	1.62	0.45
2:B:33:PRO:HD2	2:B:36:ASP:OD2	2.17	0.45
2:B:414[B]:LEU:O	2:B:417[B]:MET:HB3	2.17	0.45
1:A:303:SER:O	1:A:304:GLN:HB2	2.17	0.45
2:D:406[A]:LEU:C	2:D:407[A]:VAL:CG2	2.85	0.45
2:B:265:ARG:NH1	2:D:169:ARG:HD2	2.32	0.45
1:C:301:PRO:HG3	1:C:351:GLN:HB2	1.99	0.45
1:A:244:PRO:HG3	1:A:254:LEU:HD22	1.99	0.45
2:B:311:GLY:HA2	2:B:321:LEU:HD21	1.99	0.45
2:B:352:LEU:HG	2:B:353:ILE:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:416[B]:THR:HG23	2:B:419[B]:ARG:HB2	1.99	0.45
1:C:47:GLY:O	1:C:74:LEU:HD22	2.17	0.44
2:D:377:VAL:HG22	2:D:381:ASP:HB2	2.00	0.44
1:A:168:THR:O	1:A:214:GLY:HA3	2.18	0.44
1:C:168:THR:O	1:C:214:GLY:HA3	2.16	0.44
1:C:311:ARG:HD2	1:C:311:ARG:C	2.38	0.44
2:D:407[B]:VAL:HG23	2:D:408[B]:MET:N	2.32	0.44
2:B:287:GLY:O	2:B:312:CYS:HA	2.17	0.44
2:B:61:GLU:OE1	2:B:64:HIS:HD2	2.01	0.44
2:D:328:TYR:N	2:D:328:TYR:CD1	2.85	0.44
2:D:364:LYS:HD3	2:D:364:LYS:HA	1.64	0.44
1:C:27:GLY:HA3	1:C:148:THR:OG1	2.18	0.43
1:C:200:ARG:HB2	1:C:211:PRO:HB3	1.98	0.43
2:D:408[A]:MET:CG	4:D:526:PMR:CBA	2.96	0.43
1:A:188:LEU:CD1	1:A:199:VAL:HG22	2.48	0.43
2:B:243:ARG:NH2	2:B:261:GLU:OE1	2.50	0.43
2:D:12:PRO:HB2	2:D:122:LEU:HB3	2.00	0.43
1:C:106:LEU:HB3	1:C:138:VAL:HB	1.99	0.43
2:D:34:GLN:HG2	2:D:59:THR:HG22	2.00	0.43
1:C:116:VAL:C	1:C:118:LYS:H	2.21	0.43
2:B:273:VAL:HA	2:B:276:THR:HG23	2.00	0.43
1:A:149:THR:H	1:A:152:GLN:HE21	1.66	0.43
1:A:176:VAL:HG12	1:A:226:LEU:HD13	2.00	0.43
1:A:388:ALA:O	1:A:390:GLU:N	2.52	0.43
2:B:281:LYS:HB2	2:B:305:PHE:CD1	2.54	0.43
1:C:269:LYS:HA	1:C:269:LYS:HD2	1.76	0.43
1:C:219:PHE:HZ	1:C:230:THR:HG23	1.83	0.43
2:D:407[B]:VAL:O	2:D:409[B]:GLY:N	2.51	0.43
2:D:408[A]:MET:SD	4:D:526:PMR:HBA	2.58	0.43
2:B:418[B]:PHE:CE1	1:C:36:ARG:NH1	2.86	0.43
2:B:317:MET:C	2:B:320:PRO:HD2	2.40	0.42
2:D:161:ALA:O	2:D:191:PRO:HD2	2.18	0.42
1:A:61:VAL:HG23	2:D:410[A]:LEU:CD2	2.49	0.42
1:A:142:THR:HG21	1:A:147:ASP:OD2	2.20	0.42
1:A:409:PHE:O	1:A:412:PRO:HD2	2.19	0.42
2:B:317:MET:O	2:B:320:PRO:HD2	2.19	0.42
2:B:385:ARG:HG2	2:D:400:ASP:OD2	2.20	0.42
1:C:368:THR:HB	1:C:385:THR:HG22	2.00	0.42
2:B:178:LEU:HD12	2:B:179:LEU:N	2.34	0.42
1:C:104:ARG:HH21	1:C:135:HIS:HA	1.83	0.42
2:D:380:GLN:N	2:D:380:GLN:HE21	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:LEU:HD13	2:B:113:LEU:HD21	2.00	0.42
2:D:24:LYS:HE2	2:D:193:GLY:O	2.20	0.42
2:B:396:ASN:HB3	2:D:385:ARG:HA	2.01	0.42
1:A:47:GLY:O	1:A:73:VAL:HA	2.19	0.42
1:C:79:LEU:O	1:C:117:LEU:HD22	2.20	0.42
4:D:526:PMR:HBB	4:D:526:PMR:CHC	2.35	0.42
1:C:32:VAL:HG12	1:C:393:PHE:HZ	1.84	0.42
2:D:156:CYS:HA	2:D:205:ALA:HB1	2.01	0.42
1:A:89:LEU:O	1:A:93:VAL:HG13	2.20	0.42
2:B:356:THR:HG22	2:B:358:MET:N	2.30	0.42
2:D:37:THR:HG22	2:D:57:PHE:CD1	2.54	0.42
2:D:414[B]:LEU:HD22	2:D:418[B]:PHE:CZ	2.55	0.42
1:A:305:LEU:O	1:A:308:PRO:HD2	2.20	0.41
2:B:414[B]:LEU:CA	2:B:417[B]:MET:CB	2.67	0.41
2:D:349:ALA:HA	2:D:350:PRO:HD2	1.96	0.41
2:B:380:GLN:H	2:B:380:GLN:CD	2.24	0.41
2:B:414[B]:LEU:CD2	2:B:417[B]:MET:HG2	2.41	0.41
2:D:270:SER:HB3	2:D:399:PHE:HE1	1.85	0.41
1:C:200:ARG:NH1	1:C:200:ARG:HG3	2.32	0.41
1:C:360:HIS:HE1	1:C:368:THR:OG1	2.03	0.41
2:D:154:VAL:HA	2:D:206:HIS:CD2	2.55	0.41
1:A:270:PHE:O	1:A:274:THR:HB	2.20	0.41
1:A:35:HIS:NE2	1:A:62:MET:CE	2.83	0.41
2:D:404:HIS:O	2:D:407[B]:VAL:HG22	2.20	0.41
1:C:202:LEU:HB2	1:C:211:PRO:HG3	2.01	0.41
2:D:393:GLU:O	2:D:397:VAL:HG23	2.21	0.41
2:D:409[A]:GLY:C	4:D:526:PMR:OAD	2.59	0.41
1:A:112:CYS:HB3	2:B:96:THR:CG2	2.48	0.41
2:B:266:GLN:HG3	2:B:399:PHE:HB2	2.02	0.41
4:D:526:PMR:CBB	4:D:526:PMR:HHC	2.39	0.41
2:B:26:LEU:HD23	2:B:26:LEU:C	2.41	0.41
2:D:407[B]:VAL:CG2	2:D:408[B]:MET:N	2.83	0.41
1:A:375:ALA:HB1	2:D:273:VAL:HG21	2.02	0.41
2:D:71:ILE:O	2:D:74:LYS:HB3	2.21	0.41
1:C:304:GLN:HG3	1:C:327:PRO:HG2	2.03	0.41
1:A:188:LEU:HD11	1:A:199:VAL:HG22	2.03	0.40
1:A:53:HIS:HE1	2:B:42:LEU:HD21	1.86	0.40
2:B:410[A]:LEU:HD13	1:C:60:GLY:HA3	2.02	0.40
1:C:236:ARG:HB3	1:C:236:ARG:HE	1.50	0.40
1:A:173:LEU:HD23	1:A:218:ARG:O	2.21	0.40
1:A:301:PRO:HG3	1:A:351:GLN:HB2	2.04	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%)	384 (93%)	27 (6%)	2 (0%)	29	61
1	C	413/437 (94%)	386 (94%)	26 (6%)	1 (0%)	47	78
2	B	428/525 (82%)	402 (94%)	21 (5%)	5 (1%)	13	40
2	D	427/525 (81%)	398 (93%)	23 (5%)	6 (1%)	11	36
All	All	1681/1924 (87%)	1570 (93%)	97 (6%)	14 (1%)	22	51

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	413[A]	HIS
2	B	413[B]	HIS
1	C	343	SER
2	D	408[A]	MET
2	D	408[B]	MET
1	A	389	ILE
2	D	105	ASN
2	B	289	GLY
2	B	414[A]	LEU
2	B	414[B]	LEU
1	A	28	LEU
2	D	349	ALA
2	D	106	GLY
2	D	191	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	329/344 (96%)	294 (89%)	35 (11%)	6	20
1	C	330/344 (96%)	291 (88%)	39 (12%)	5	16
2	B	347/417 (83%)	313 (90%)	34 (10%)	8	24
2	D	345/417 (83%)	313 (91%)	32 (9%)	9	27
All	All	1351/1522 (89%)	1211 (90%)	140 (10%)	7	21

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	15	VAL
1	A	19	ARG
1	A	21	GLN
1	A	37	LYS
1	A	61	VAL
1	A	66	GLU
1	A	73	VAL
1	A	74	LEU
1	A	77	GLN
1	A	82	LEU
1	A	93	VAL
1	A	98	GLU
1	A	100	ARG
1	A	104	ARG
1	A	118	LYS
1	A	121	LEU
1	A	123	ARG
1	A	131	LEU
1	A	137	ARG
1	A	138	VAL
1	A	173	LEU
1	A	188	LEU
1	A	196	VAL
1	A	256	LEU
1	A	292	LEU
1	A	329	LEU
1	A	357	LEU

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Mol	Chain	Res	Type
1	A	372	LEU
1	A	378	LEU
1	A	404	ASP
1	A	411	ARG
1	A	416	ARG
1	A	418	LEU
1	A	419	LEU
2	B	52	ARG
2	B	61	GLU
2	B	96	THR
2	B	100	LEU
2	B	101	GLN
2	B	105	ASN
2	B	111	LEU
2	B	121	GLU
2	B	124	SER
2	B	142	ARG
2	B	151	THR
2	B	159	LEU
2	B	164	LEU
2	B	168	HIS
2	B	181	THR
2	B	210	LEU
2	B	221	ARG
2	B	266	GLN
2	B	274	ASP
2	B	279	THR
2	B	288	ASP
2	B	315	ARG
2	B	316	GLU
2	B	330	LEU
2	B	333	LEU
2	B	356	THR
2	B	372	VAL
2	B	377	VAL
2	B	385	ARG
2	B	400	ASP
2	B	408[A]	MET
2	B	408[B]	MET
2	B	416[B]	THR
2	B	419[B]	ARG
1	C	7	THR

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Mol	Chain	Res	Type
1	C	11	THR
1	C	15	VAL
1	C	28	LEU
1	C	36	ARG
1	C	56	GLN
1	C	73	VAL
1	C	74	LEU
1	C	76	GLU
1	C	77	GLN
1	C	82	LEU
1	C	88	GLU
1	C	100	ARG
1	C	121	LEU
1	C	128	LEU
1	C	131	LEU
1	C	138	VAL
1	C	142	THR
1	C	173	LEU
1	C	188	LEU
1	C	192	THR
1	C	196	VAL
1	C	199	VAL
1	C	200	ARG
1	C	201	MET
1	C	213	VAL
1	C	228[A]	GLU
1	C	228[B]	GLU
1	C	236	ARG
1	C	249	GLU
1	C	269	LYS
1	C	274	THR
1	C	280	ARG
1	C	292	LEU
1	C	329	LEU
1	C	361	GLU
1	C	372	LEU
1	C	378	LEU
1	C	408	LEU
2	D	25	ASP
2	D	26	LEU
2	D	58	SER
2	D	61	GLU

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Mol	Chain	Res	Type
2	D	94	THR
2	D	100	LEU
2	D	101	GLN
2	D	105	ASN
2	D	120	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	227	CYS
2	D	263	THR
2	D	264	LEU
2	D	266	GLN
2	D	273	VAL
2	D	279	THR
2	D	315	ARG
2	D	319	ARG
2	D	328	TYR
2	D	330	LEU
2	D	346	GLU
2	D	360	ARG
2	D	364	LYS
2	D	380	GLN
2	D	385	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	A	351	GLN
2	B	13	HIS
2	B	34	GLN
2	B	64	HIS
2	B	157	ASN
2	B	168	HIS
2	B	204	GLN
2	B	229	GLN
2	B	266	GLN

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Mol	Chain	Res	Type
2	B	404	HIS
1	C	105	GLN
1	C	152	GLN
1	C	304	GLN
1	C	360	HIS
1	C	376	ASN
2	D	13	HIS
2	D	31	HIS
2	D	34	GLN
2	D	112	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	357	GLN
2	D	380	GLN

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 carbohydrates 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	$\# Z > 2$
3	SF4	A	425	1,2	0,12,12	0.00	-	-		
4	PMR	D	526	5	37,53,53	4.86	21 (56%)	20,89,89	2.24	6 (30%)
3	SF4	C	425	1,2	0,12,12	0.00	-	-		
4	PMR	B	526	5	37,53,53	4.84	23 (62%)	20,89,89	2.26	8 (40%)

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	-	-	0/6/5/5
4	PMR	D	526	5	-	6/11/131/131	-
3	SF4	C	425	1,2	-	-	0/6/5/5
4	PMR	B	526	5	-	4/11/131/131	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	526	PMR	CHA-C1A	-12.26	1.37	1.53
4	D	526	PMR	CHA-C1A	-11.97	1.38	1.53
4	D	526	PMR	CHD-C1D	-10.51	1.36	1.53
4	B	526	PMR	CHD-C1D	-10.06	1.37	1.53
4	D	526	PMR	CHD-C4C	-9.49	1.37	1.53
4	B	526	PMR	CHD-C4C	-9.22	1.37	1.53
4	B	526	PMR	C4D-ND	-7.85	1.33	1.50
4	D	526	PMR	C4D-ND	-7.83	1.33	1.50
4	D	526	PMR	C2D-C1D	-7.82	1.39	1.53
4	B	526	PMR	C2D-C1D	-7.50	1.39	1.53
4	D	526	PMR	C1D-ND	-7.16	1.35	1.50
4	B	526	PMR	C1D-ND	-7.11	1.35	1.50
4	D	526	PMR	C3D-C2D	-6.96	1.37	1.55
4	B	526	PMR	C3D-C2D	-6.94	1.37	1.55
4	D	526	PMR	C3D-CAD	-6.86	1.38	1.51
4	B	526	PMR	C3D-CAD	-6.64	1.39	1.51
4	B	526	PMR	CHB-C4A	-6.30	1.37	1.53
4	D	526	PMR	CHB-C4A	-6.14	1.37	1.53
4	B	526	PMR	CHC-C1C	-5.87	1.38	1.53
4	D	526	PMR	CHC-C1C	-5.83	1.38	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	526	PMR	CHB-C1B	-5.65	1.37	1.51
4	D	526	PMR	CHB-C1B	-5.64	1.37	1.51
4	D	526	PMR	CHC-C4B	-5.47	1.37	1.51
4	B	526	PMR	CHC-C4B	-5.40	1.38	1.51
4	B	526	PMR	C4A-C3A	-4.37	1.37	1.50
4	D	526	PMR	C4A-C3A	-4.17	1.38	1.50
4	B	526	PMR	C1C-C2C	-3.87	1.39	1.50
4	D	526	PMR	C1C-C2C	-3.86	1.39	1.50
4	B	526	PMR	C2C-C3C	3.86	1.37	1.34
4	D	526	PMR	C4C-C3C	-3.84	1.39	1.50
4	B	526	PMR	C4C-C3C	-3.78	1.39	1.50
4	B	526	PMR	C1A-C2A	-3.68	1.39	1.50
4	B	526	PMR	C3B-CAB	-3.65	1.40	1.47
4	D	526	PMR	C3B-CAB	-3.57	1.40	1.47
4	D	526	PMR	C2C-C3C	3.47	1.36	1.34
4	B	526	PMR	C3A-C2A	3.46	1.36	1.34
4	D	526	PMR	C1A-C2A	-3.46	1.40	1.50
4	D	526	PMR	C3A-C2A	3.46	1.36	1.34
4	B	526	PMR	C3B-C2B	-2.61	1.36	1.40
4	D	526	PMR	C3B-C2B	-2.53	1.36	1.40
4	D	526	PMR	CMA-C3A	2.45	1.54	1.50
4	B	526	PMR	CAA-C2A	2.19	1.54	1.51
4	B	526	PMR	CMC-C2C	2.10	1.53	1.50
4	B	526	PMR	CMA-C3A	2.04	1.53	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	526	PMR	C1D-CHD-C4C	5.54	124.18	112.37
4	D	526	PMR	C1D-CHD-C4C	5.39	123.86	112.37
4	D	526	PMR	CMD-C2D-C3D	4.46	125.37	114.29
4	B	526	PMR	CMD-C2D-C3D	4.14	124.56	114.29
4	D	526	PMR	O2D-CGD-CBD	3.30	118.87	111.11
4	B	526	PMR	O2D-CGD-CBD	3.18	118.57	111.11
4	D	526	PMR	O1D-CGD-CBD	-2.74	119.11	124.54
4	B	526	PMR	CHB-C1B-C2B	-2.61	124.93	129.45
4	D	526	PMR	CBA-CAA-C2A	-2.50	109.92	114.35
4	B	526	PMR	O1D-CGD-CBD	-2.32	119.94	124.54
4	B	526	PMR	CBC-CAC-C3C	2.30	116.47	112.98
4	D	526	PMR	CHB-C1B-C2B	-2.25	125.55	129.45
4	B	526	PMR	C4D-C3D-CAD	2.05	109.39	104.73
4	B	526	PMR	CBA-CAA-C2A	-2.04	110.73	114.35

There are no chirality outliers.

All (10) torsion outliers are listed below:

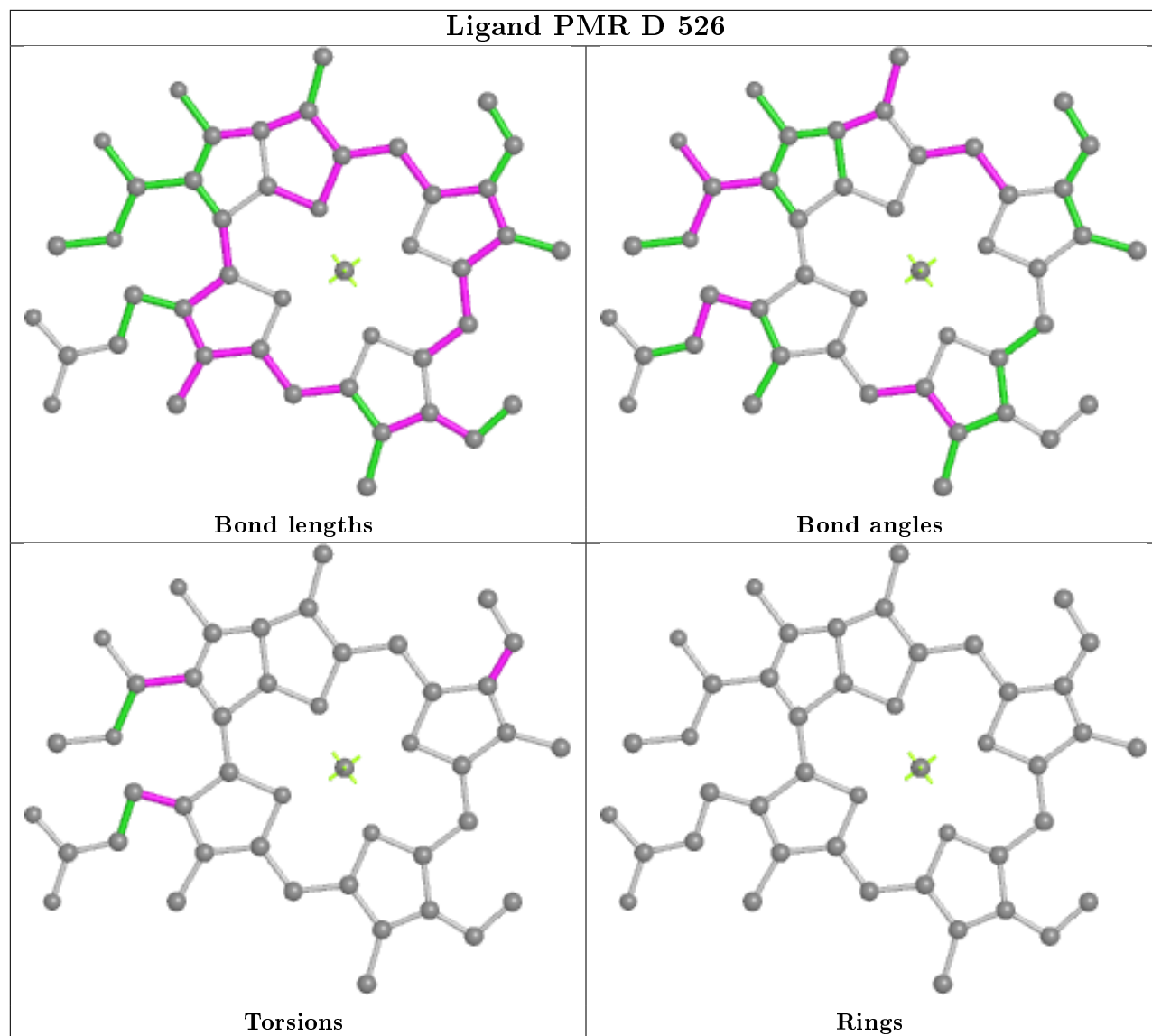
Mol	Chain	Res	Type	Atoms
4	D	526	PMR	C1A-C2A-CAA-CBA
4	B	526	PMR	C2C-C3C-CAC-CBC
4	B	526	PMR	C4C-C3C-CAC-CBC
4	D	526	PMR	C4C-C3C-CAC-CBC
4	D	526	PMR	C2C-C3C-CAC-CBC
4	B	526	PMR	C2A-CAA-CBA-CGA
4	B	526	PMR	C3A-C2A-CAA-CBA
4	D	526	PMR	CHA-CBD-CGD-O2D
4	D	526	PMR	C3A-C2A-CAA-CBA
4	D	526	PMR	CHA-CBD-CGD-O1D

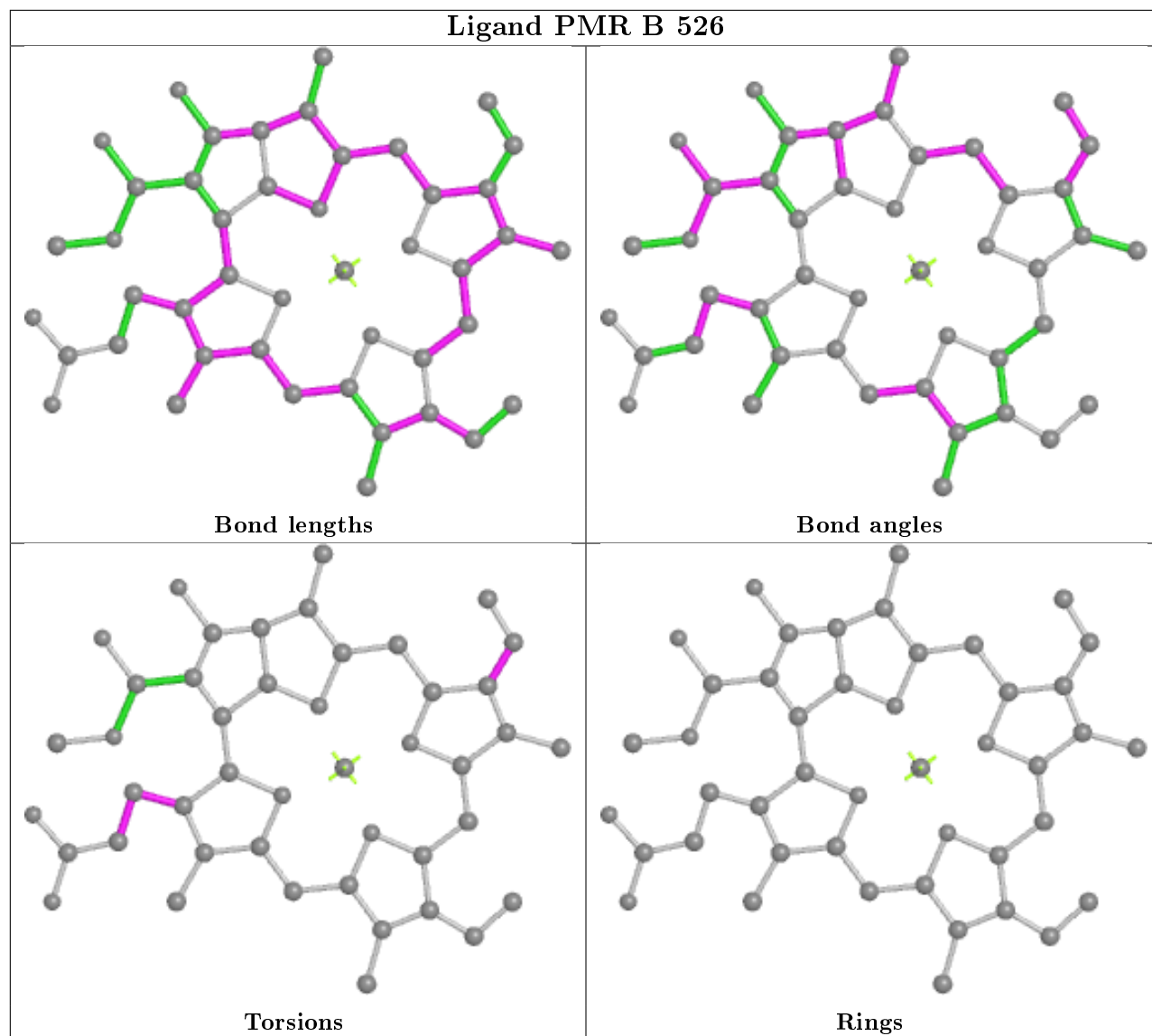
There are no ring outliers.

3 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	526	PMR	18	0
3	C	425	SF4	1	0
4	B	526	PMR	9	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 than 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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	415/437 (94%)	0.04	0 100 100	41, 52, 64, 69	0
1	C	414/437 (94%)	0.02	2 (0%) 91 91	40, 52, 64, 69	0
2	B	419/525 (79%)	0.03	12 (2%) 51 47	39, 47, 54, 64	5 (1%)
2	D	419/525 (79%)	0.03	11 (2%) 56 52	39, 47, 55, 65	6 (1%)
All	All	1667/1924 (86%)	0.03	25 (1%) 73 73	39, 49, 60, 69	11 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	413[A]	HIS	5.1
2	B	413[A]	HIS	3.6
2	B	416[B]	THR	3.4
2	D	409[A]	GLY	3.1
2	B	408[A]	MET	3.0
2	D	417[B]	MET	3.0
2	D	412[A]	GLU	2.9
2	B	347	ALA	2.9
2	B	409[A]	GLY	2.9
2	D	408[A]	MET	2.8
2	B	188	VAL	2.8
2	D	410[A]	LEU	2.8
1	C	7	THR	2.6
2	B	410[A]	LEU	2.4
2	B	146	VAL	2.4
2	B	156	CYS	2.2
2	D	206	HIS	2.2
2	B	201	LYS	2.2
2	B	414[A]	LEU	2.1
2	D	146	VAL	2.1
2	D	207	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	418[B]	PHE	2.1
1	C	123	ARG	2.0
2	B	205	ALA	2.0
2	D	141	VAL	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](#)

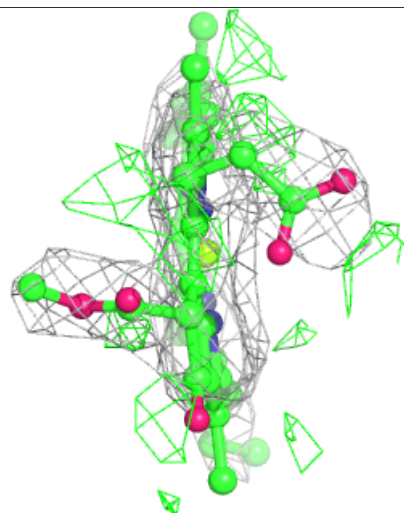
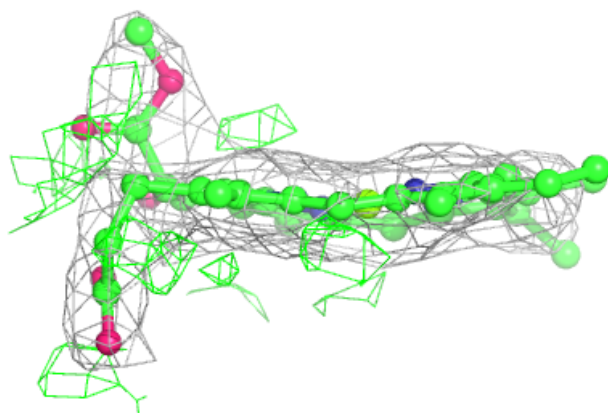
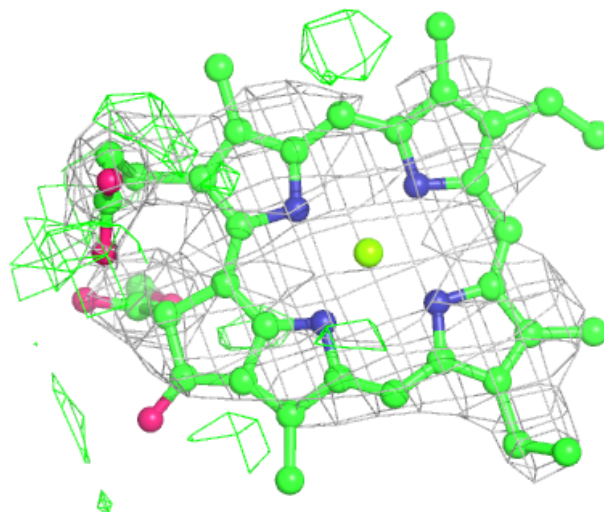
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PMR	D	526	45/45	0.85	0.44	23,26,27,28	45
4	PMR	B	526	45/45	0.93	0.37	15,18,23,26	45
3	SF4	A	425	8/8	0.98	0.13	31,33,33,34	0
3	SF4	C	425	8/8	0.99	0.12	33,34,35,36	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.

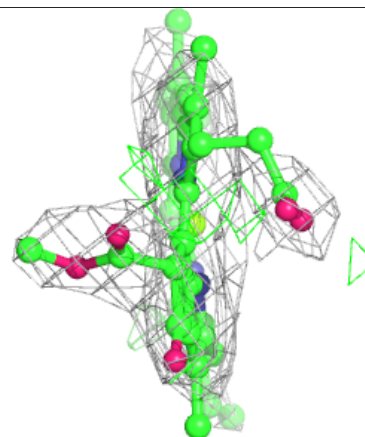
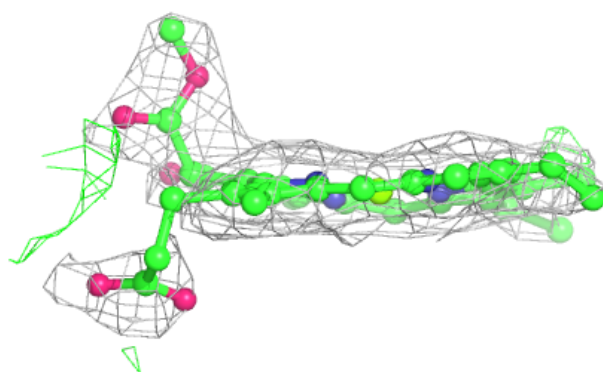
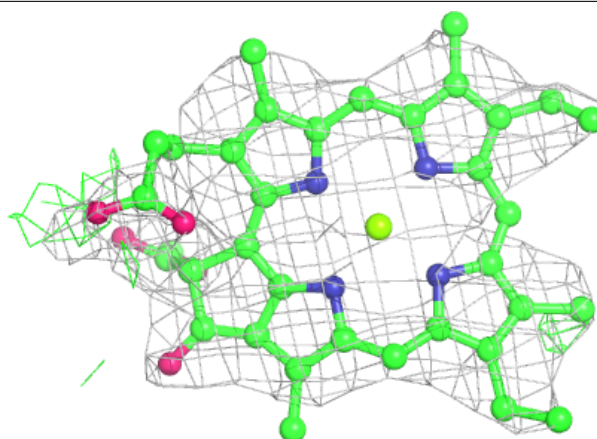
Electron density around PMR D 526:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.