



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:26 am GMT

PDB ID : 3AET
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 : 2.91 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

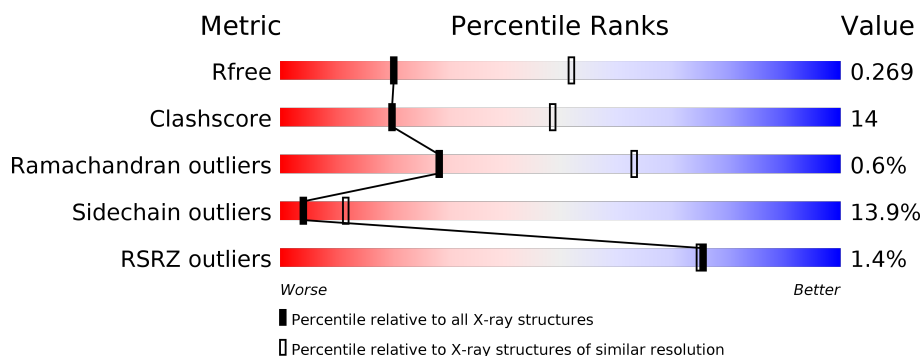
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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}	100719	1813 (2.94-2.90)
Clashscore	112137	2045 (2.94-2.90)
Ramachandran outliers	110173	1997 (2.94-2.90)
Sidechain outliers	110143	1999 (2.94-2.90)
RSRZ outliers	101464	1825 (2.94-2.90)

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. 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	436	<div> <div> <div>2%</div> <div>62%</div> <div>29%</div> <div>5%</div> </div> </div>
1	C	436	<div> <div>64%</div> <div>26%</div> <div>5%</div> </div>
2	B	525	<div> <div>2%</div> <div>54%</div> <div>22%</div> <div>20%</div> </div>
2	D	525	<div> <div>54%</div> <div>22%</div> <div>20%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SF4	C	425	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12782 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	0	0
			3160	2005	557	583	15			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	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	MET	-	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

Continued on next page...

Continued from previous page...

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

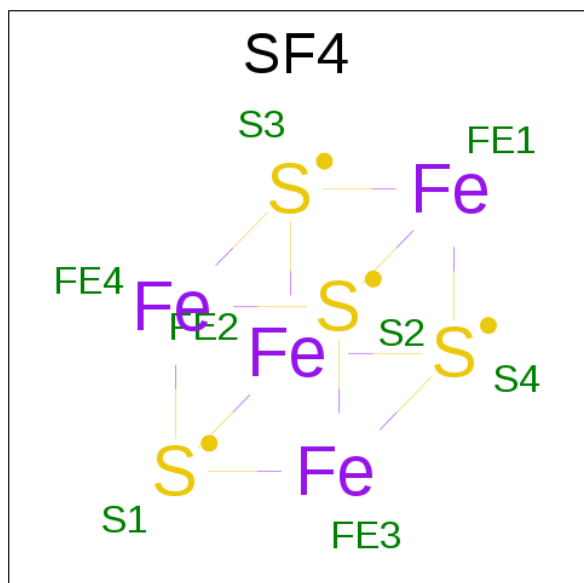
- Molecule 2 is a protein called Light-independent protochlorophyllide reductase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	0	0	0
			3218	2048	557	591	22			
2	D	420	Total	C	N	O	S	0	0	0
			3218	2048	557	591	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	36	CYS	ASP	ENGINEERED	UNP P26163
D	36	CYS	ASP	ENGINEERED	UNP P26163

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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		

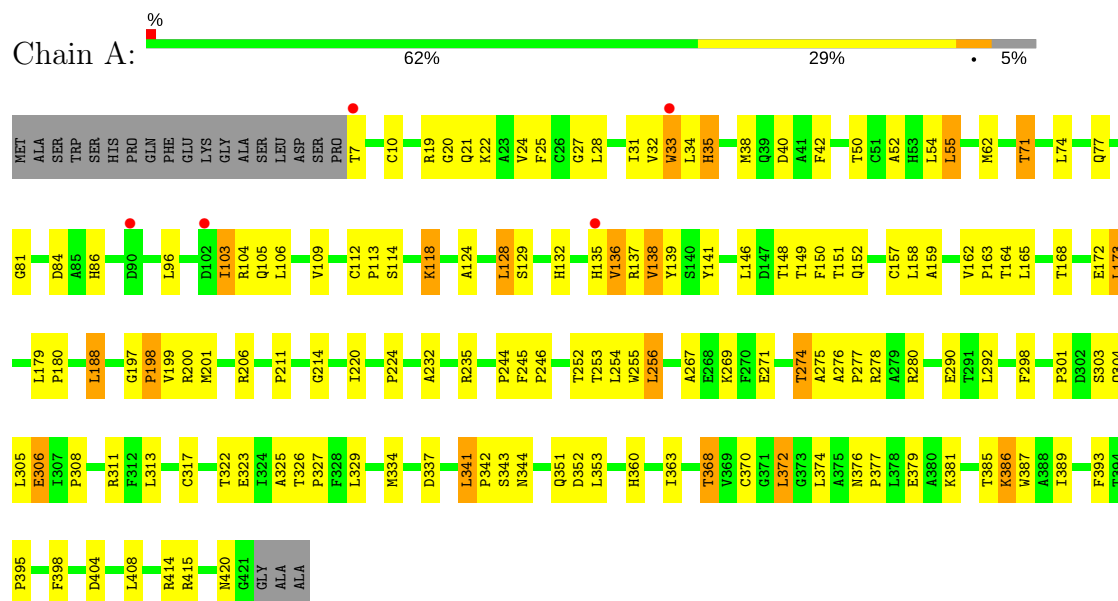
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	O 2	0	0
4	C	1	Total 1	O 1	0	0
4	D	3	Total 3	O 3	0	0

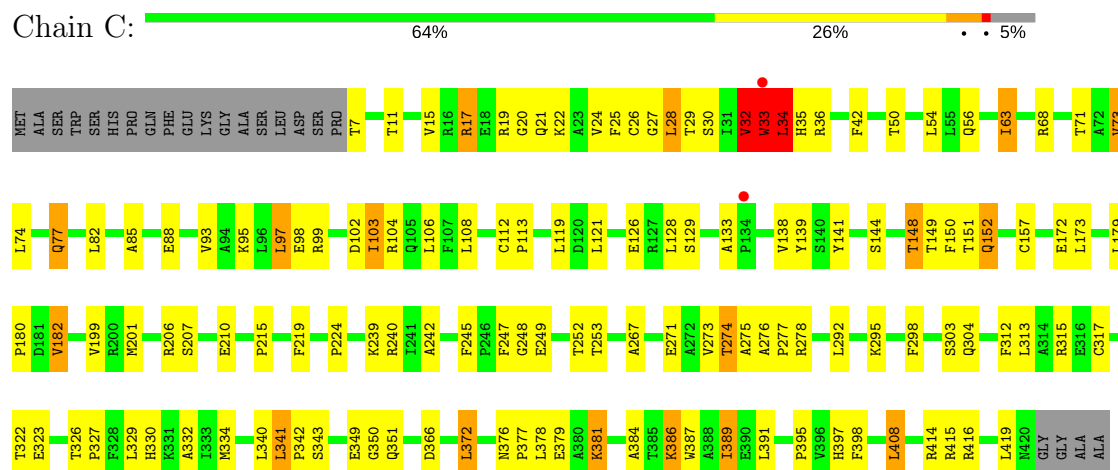
3 Residue-property plots

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

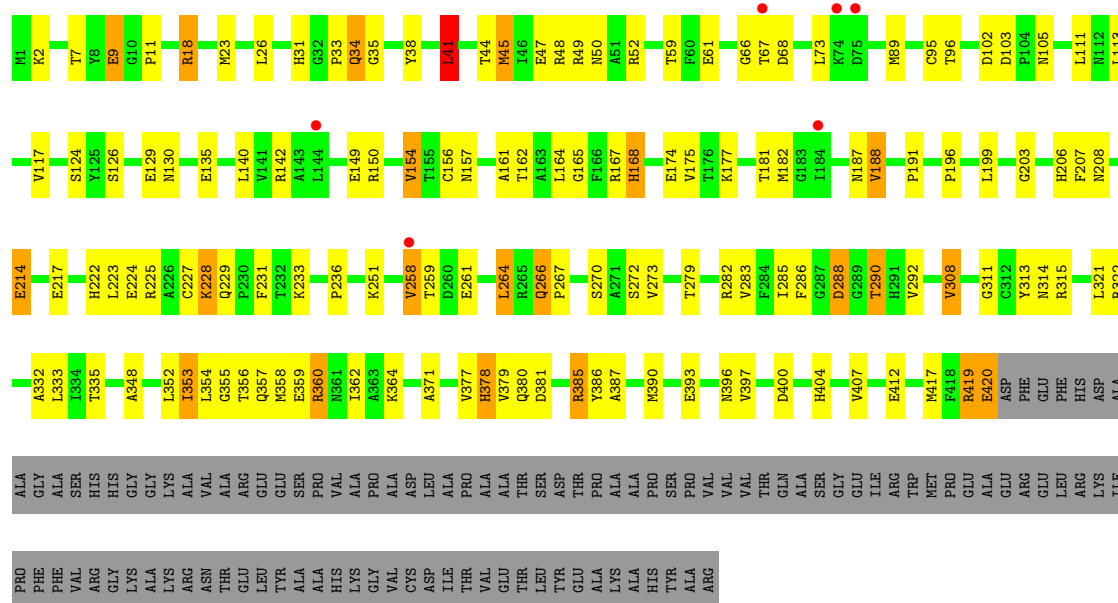


- Molecule 1: Light-independent protochlorophyllide reductase subunit N



- Molecule 2: Light-independent protochlorophyllide reductase subunit B





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.44Å 81.44Å 95.86Å 102.53° 110.89° 94.44°	Depositor
Resolution (Å)	40.05 – 2.91 40.05 – 2.91	Depositor EDS
% Data completeness (in resolution range)	89.0 (40.05-2.91) 82.5 (40.05-2.91)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.211 , 0.275 0.212 , 0.269	Depositor DCC
R_{free} test set	2171 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	63.7	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12782	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.33% 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

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	0.52	0/3227	0.68	0/4382
1	C	0.51	0/3223	0.72	2/4377 (0.0%)
2	B	0.54	0/3289	0.71	1/4476 (0.0%)
2	D	0.58	1/3289 (0.0%)	0.71	2/4476 (0.0%)
All	All	0.54	1/13028 (0.0%)	0.70	5/17711 (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
1	A	0	1
1	C	0	1
2	D	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	228	LYS	CG-CD	5.86	1.72	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	34	LEU	CA-CB-CG	8.44	134.71	115.30
1	C	33	TRP	N-CA-C	-7.33	91.20	111.00
2	B	178	LEU	CA-CB-CG	6.36	129.93	115.30
2	D	314	ASN	N-CA-CB	-5.37	100.93	110.60
2	D	41	LEU	CA-CB-CG	5.30	127.49	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	GLY	Peptide
1	C	32	VAL	Peptide
2	D	419	ARG	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	96	0
1	C	3160	0	3196	93	0
2	B	3218	0	3245	106	0
2	D	3218	0	3245	98	0
3	A	8	0	0	0	0
3	C	8	0	0	2	0
4	A	2	0	0	0	0
4	C	1	0	0	1	0
4	D	3	0	0	0	0
All	All	12782	0	12885	365	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (365) 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:360:ARG:HH11	2:B:360:ARG:HG3	1.15	1.07
2:B:380:GLN:NE2	2:D:404:HIS:ND1	2.16	0.93
2:D:360:ARG:HG3	2:D:360:ARG:HH11	1.33	0.93
1:A:341:LEU:HD23	1:A:342:PRO:HD2	1.50	0.93
1:A:34:LEU:HD22	1:A:38:MET:CE	2.02	0.89
1:C:389:ILE:H	1:C:389:ILE:HD12	1.41	0.85
2:B:162:THR:H	2:B:168:HIS:HD2	1.25	0.83
2:D:59:THR:HG22	2:D:59:THR:O	1.76	0.83
2:D:214:GLU:OE2	2:D:290:THR:HB	1.79	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:THR:HG21	1:A:363:ILE:HG21	1.62	0.81
2:B:360:ARG:NH1	2:B:360:ARG:HG3	1.94	0.80
1:A:276:ALA:HB3	1:A:277:PRO:HD3	1.64	0.79
2:B:18:ARG:HH11	2:B:18:ARG:HG2	1.46	0.79
1:A:377:PRO:HA	2:B:50:ASN:O	1.82	0.79
2:D:356:THR:HB	2:D:359:GLU:OE2	1.82	0.79
2:D:264:LEU:HD22	2:D:267:PRO:HD3	1.65	0.79
2:B:378:HIS:CE1	2:B:380:GLN:HB2	2.19	0.78
2:D:353:ILE:HD11	2:D:359:GLU:HB3	1.64	0.78
1:C:27:GLY:H	1:C:148:THR:HG23	1.49	0.78
1:A:34:LEU:HD22	1:A:38:MET:HE1	1.65	0.78
2:B:360:ARG:HH11	2:B:360:ARG:CG	1.94	0.78
2:D:161:ALA:O	2:D:191:PRO:HD2	1.85	0.74
2:B:103:ASP:O	2:B:107:ILE:HG12	1.87	0.74
1:A:42:PHE:HB2	1:A:103:ILE:HG13	1.71	0.73
1:A:165:LEU:HD22	1:A:211:PRO:O	1.88	0.73
2:B:17:MET:CE	2:B:39:ALA:HB3	2.19	0.73
1:C:112:CYS:HB2	1:C:113:PRO:HD3	1.71	0.72
2:D:162:THR:H	2:D:168:HIS:HD2	1.35	0.72
2:B:380:GLN:HA	2:B:380:GLN:OE1	1.91	0.71
1:A:33:TRP:CH2	1:A:151:THR:HG22	2.25	0.71
1:A:253:THR:OG1	1:A:278:ARG:HD3	1.90	0.70
1:A:33:TRP:HH2	1:A:151:THR:HG22	1.57	0.70
2:B:273:VAL:H	1:C:376:ASN:HD21	1.40	0.69
1:C:377:PRO:HA	2:D:50:ASN:O	1.92	0.69
1:C:267:ALA:O	1:C:271:GLU:HG2	1.92	0.69
1:C:42:PHE:HB2	1:C:103:ILE:HG13	1.75	0.69
1:C:28:LEU:HD22	3:C:425:SF4:S2	2.33	0.68
1:A:149:THR:HB	1:A:152:GLN:NE2	2.09	0.68
1:A:50:THR:HA	2:B:11:PRO:HG3	1.74	0.68
2:D:31:HIS:CD2	2:D:73:LEU:HB2	2.29	0.67
2:D:353:ILE:HD12	2:D:354:LEU:N	2.09	0.67
1:A:306:GLU:HG3	1:A:325:ALA:O	1.95	0.66
1:C:33:TRP:CD1	1:C:34:LEU:N	2.64	0.66
1:A:27:GLY:HA3	1:A:148:THR:CG2	2.25	0.66
1:A:34:LEU:HD22	1:A:38:MET:HE2	1.78	0.66
1:C:50:THR:HA	2:D:11:PRO:HG3	1.77	0.66
1:C:215:PRO:O	1:C:239:LYS:NZ	2.28	0.66
2:D:282:ARG:CZ	2:D:308:VAL:HG21	2.26	0.66
1:C:298:PHE:CE1	1:C:323:GLU:HB3	2.31	0.65
2:B:161:ALA:O	2:B:191:PRO:HD2	1.95	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:ARG:HD2	2:B:164:LEU:HB2	1.78	0.65
2:B:243:ARG:NH2	2:B:261:GLU:OE2	2.30	0.65
1:C:276:ALA:HB3	1:C:277:PRO:HD3	1.80	0.64
1:A:31:ILE:HD11	1:A:109:VAL:HG21	1.78	0.64
2:D:23:MET:SD	2:D:26:LEU:HD13	2.38	0.64
2:B:380:GLN:HE21	2:D:404:HIS:CE1	2.16	0.64
2:B:175:VAL:HG21	2:B:390:MET:HE3	1.80	0.64
2:B:123:PRO:HG2	2:B:127:ARG:HG2	1.81	0.63
1:A:415:ARG:HD2	2:D:279:THR:OG1	1.98	0.62
2:B:285:ILE:HG22	2:B:292:VAL:HG13	1.81	0.62
1:C:274:THR:O	1:C:278:ARG:HG3	2.00	0.62
1:A:27:GLY:HA3	1:A:148:THR:HG21	1.81	0.62
1:C:341:LEU:HD23	1:C:342:PRO:HD2	1.80	0.62
2:D:282:ARG:NH2	2:D:308:VAL:HG21	2.15	0.62
1:C:33:TRP:CH2	1:C:151:THR:HG22	2.35	0.62
2:D:59:THR:CG2	2:D:59:THR:O	2.47	0.62
2:B:360:ARG:NH1	2:B:360:ARG:CG	2.57	0.61
2:B:277:TYR:O	2:B:281:LYS:NZ	2.22	0.61
1:A:313:LEU:O	1:A:317:CYS:HB2	1.99	0.61
2:B:157:ASN:ND2	2:B:188:VAL:HG22	2.15	0.61
2:B:135:GLU:HA	2:B:135:GLU:OE1	2.00	0.61
1:A:33:TRP:C	1:A:33:TRP:CD1	2.74	0.60
1:C:129:SER:O	1:C:133:ALA:HB2	2.00	0.60
1:C:33:TRP:C	1:C:33:TRP:CD1	2.75	0.60
2:B:319:ARG:HG2	2:B:320:PRO:HD3	1.84	0.60
2:B:33:PRO:HD2	2:B:94:THR:HG21	1.83	0.60
2:B:31:HIS:CD2	2:B:73:LEU:HB2	2.36	0.60
1:A:159:ALA:O	1:A:163:PRO:HD3	2.02	0.59
2:B:286:PHE:O	2:B:355:GLY:HA2	2.02	0.59
1:A:224:PRO:HA	1:A:245:PHE:CZ	2.37	0.59
2:D:9:GLU:OE2	2:D:130:ASN:HB2	2.02	0.59
2:B:17:MET:HE1	2:B:39:ALA:HB3	1.84	0.59
1:A:188:LEU:HD22	1:A:201:MET:HE3	1.85	0.59
2:D:264:LEU:HD22	2:D:267:PRO:CD	2.31	0.58
2:D:214:GLU:OE2	2:D:290:THR:CB	2.49	0.58
1:C:27:GLY:N	1:C:148:THR:HG23	2.17	0.58
1:C:249:GLU:OE2	1:C:278:ARG:HD2	2.03	0.58
2:D:236:PRO:HG2	2:D:390:MET:HG2	1.86	0.58
1:A:188:LEU:HD22	1:A:201:MET:CE	2.34	0.58
2:D:223:LEU:HD13	2:D:229:GLN:HE22	1.69	0.58
1:A:22:LYS:H	2:B:59:THR:HG21	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ARG:HH11	1:C:36:ARG:HG2	1.68	0.58
1:A:19:ARG:HG2	1:A:20:GLY:H	1.68	0.57
2:B:47:GLU:O	2:B:48:ARG:HB3	2.05	0.57
2:B:31:HIS:HA	2:B:58:SER:OG	2.04	0.57
1:C:33:TRP:HH2	1:C:151:THR:HG22	1.66	0.57
2:B:18:ARG:HG2	2:B:18:ARG:NH1	2.14	0.57
1:A:52:ALA:HA	1:A:71:THR:HG21	1.85	0.57
1:A:274:THR:O	1:A:278:ARG:HG3	2.05	0.57
2:B:17:MET:HE3	2:B:39:ALA:HB3	1.87	0.57
1:A:25:PHE:HZ	2:B:41:LEU:HD21	1.69	0.57
2:D:286:PHE:O	2:D:355:GLY:HA2	2.05	0.57
1:A:137:ARG:HH12	1:A:164:THR:HB	1.70	0.57
2:B:157:ASN:HD22	2:B:188:VAL:HG22	1.70	0.57
1:A:271:GLU:O	1:A:275:ALA:HB2	2.05	0.57
2:B:48:ARG:O	2:B:48:ARG:HG3	2.04	0.56
2:D:285:ILE:HG22	2:D:292:VAL:HG13	1.87	0.56
2:D:95:CYS:HB3	2:D:124:SER:OG	2.05	0.56
2:B:162:THR:N	2:B:168:HIS:HD2	2.01	0.56
2:D:154:VAL:HA	2:D:206:HIS:CE1	2.39	0.56
2:D:358:MET:HE2	2:D:362:ILE:CG1	2.36	0.56
1:C:25:PHE:CD2	1:C:29:THR:HG21	2.41	0.56
1:A:149:THR:H	1:A:152:GLN:NE2	2.03	0.56
2:B:282:ARG:NH1	2:B:348:ALA:O	2.37	0.56
2:D:378:HIS:CE1	2:D:380:GLN:HG2	2.40	0.56
1:C:207:SER:O	1:C:210:GLU:HG2	2.06	0.56
1:C:25:PHE:HD2	1:C:29:THR:HG21	1.71	0.56
2:D:356:THR:HG22	2:D:358:MET:H	1.71	0.56
2:B:288:ASP:C	2:B:288:ASP:OD2	2.45	0.55
2:B:171:ASP:CG	2:B:390:MET:HG3	2.27	0.55
1:C:27:GLY:H	1:C:148:THR:CG2	2.19	0.55
2:B:154:VAL:HA	2:B:206:HIS:CE1	2.41	0.55
1:C:33:TRP:CD1	1:C:34:LEU:HB3	2.41	0.55
1:C:372:LEU:HD13	1:C:387:TRP:HB2	1.87	0.55
1:A:376:ASN:ND2	2:D:273:VAL:HG23	2.21	0.55
2:B:174:GLU:OE1	2:B:177:LYS:HE2	2.06	0.55
1:C:19:ARG:HD3	1:C:20:GLY:H	1.70	0.55
2:B:279:THR:OG1	1:C:415:ARG:HD2	2.07	0.55
1:C:224:PRO:HA	1:C:245:PHE:CZ	2.41	0.55
1:A:149:THR:HB	1:A:152:GLN:HE22	1.72	0.55
2:B:319:ARG:CG	2:B:320:PRO:HD3	2.36	0.55
2:B:18:ARG:HG2	2:B:163:ALA:O	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:9:GLU:HG2	2:D:129:GLU:HB3	1.88	0.55
2:D:313:TYR:HA	2:D:335:THR:O	2.06	0.55
1:C:384:ALA:HB2	1:C:416:ARG:HD3	1.88	0.54
2:D:264:LEU:CD2	2:D:267:PRO:HD3	2.36	0.54
2:B:34:GLN:HA	2:B:59:THR:HG22	1.88	0.54
1:C:149:THR:H	1:C:152:GLN:HE21	1.55	0.54
2:B:26:LEU:HD12	2:B:196:PRO:HG3	1.89	0.54
1:C:372:LEU:O	2:D:44:THR:HG21	2.08	0.54
2:D:34:GLN:HB2	2:D:59:THR:HG23	1.90	0.53
1:C:271:GLU:O	1:C:275:ALA:HB2	2.08	0.53
2:B:385:ARG:HH12	2:D:387:ALA:HB2	1.73	0.53
2:B:393:GLU:O	2:B:397:VAL:HG23	2.08	0.53
2:D:377:VAL:HG22	2:D:381:ASP:HB2	1.89	0.53
1:C:240:ARG:HH21	1:C:242:ALA:HA	1.73	0.53
2:B:360:ARG:HG2	2:B:370:CYS:SG	2.49	0.53
1:C:56:GLN:HA	1:C:63:ILE:HD13	1.90	0.53
2:D:378:HIS:CD2	2:D:379:VAL:HG12	2.43	0.53
1:A:137:ARG:HG3	1:A:139:TYR:CE2	2.44	0.53
2:D:182:MET:HA	2:D:258:VAL:HG23	1.90	0.53
2:B:33:PRO:HG2	2:B:36:CYS:HB2	1.91	0.53
2:D:26:LEU:HD12	2:D:196:PRO:HG3	1.91	0.53
1:A:106:LEU:HB3	1:A:138:VAL:HB	1.90	0.52
2:D:393:GLU:O	2:D:397:VAL:HG23	2.09	0.52
1:A:341:LEU:CD2	1:A:342:PRO:HD2	2.32	0.52
1:C:239:LYS:HD2	1:C:239:LYS:N	2.25	0.52
1:C:30:SER:HA	1:C:33:TRP:CE3	2.44	0.51
2:B:89:MET:HB2	2:B:117:VAL:HG22	1.92	0.51
1:A:86:HIS:CE1	1:A:124:ALA:HB2	2.46	0.51
2:B:385:ARG:HD2	2:D:385:ARG:NH1	2.25	0.51
1:C:33:TRP:HD1	1:C:33:TRP:C	2.13	0.51
1:A:301:PRO:HG2	1:A:351:GLN:OE1	2.11	0.51
2:D:89:MET:HB2	2:D:117:VAL:HG22	1.91	0.51
2:D:377:VAL:CG2	2:D:381:ASP:HB2	2.40	0.51
2:B:165:GLY:HA3	2:B:168:HIS:CG	2.46	0.51
2:B:357:GLN:NE2	2:B:360:ARG:HH12	2.10	0.50
1:A:137:ARG:HH12	1:A:164:THR:CB	2.24	0.50
1:A:387:TRP:CZ3	1:A:389:ILE:HB	2.46	0.50
2:B:167:ARG:HD2	2:B:387:ALA:O	2.12	0.50
2:D:322:ARG:HG2	2:D:332:ALA:HB3	1.93	0.50
2:D:162:THR:HG22	2:D:191:PRO:HG2	1.94	0.50
2:D:360:ARG:O	2:D:364:LYS:HG2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:PHE:HB3	1:A:368:THR:HG23	1.93	0.50
2:B:171:ASP:HB3	2:B:390:MET:HE1	1.94	0.49
1:C:42:PHE:HB2	1:C:103:ILE:CG1	2.41	0.49
2:D:360:ARG:HG3	2:D:360:ARG:NH1	2.11	0.49
2:D:66:GLY:C	2:D:68:ASP:H	2.15	0.49
2:B:264:LEU:HD22	2:B:267:PRO:HD3	1.95	0.49
2:D:167:ARG:HD2	2:D:387:ALA:O	2.12	0.49
2:D:157:ASN:HD22	2:D:188:VAL:HG13	1.78	0.49
2:D:358:MET:HE2	2:D:362:ILE:HG12	1.94	0.49
1:A:112:CYS:SG	1:A:146:LEU:HG	2.52	0.49
2:B:266:GLN:HE21	2:B:267:PRO:N	2.11	0.49
1:A:389:ILE:H	1:A:389:ILE:HD12	1.77	0.49
1:A:33:TRP:HZ3	1:A:150:PHE:CE1	2.30	0.48
1:A:305:LEU:O	1:A:308:PRO:HD2	2.13	0.48
2:B:33:PRO:HD3	2:B:96:THR:HB	1.95	0.48
1:C:144:SER:O	1:C:148:THR:HG22	2.13	0.48
1:C:271:GLU:OE1	1:C:271:GLU:HA	2.13	0.48
1:C:322:THR:OG1	1:C:323:GLU:N	2.46	0.48
2:B:126:SER:O	2:B:127:ARG:HD2	2.12	0.48
2:B:165:GLY:HA3	2:B:168:HIS:CD2	2.49	0.48
1:A:180:PRO:HG2	1:A:395:PRO:HA	1.95	0.48
1:C:141:TYR:CZ	1:C:157:CYS:HB2	2.48	0.48
1:A:112:CYS:HB2	1:A:113:PRO:HD3	1.95	0.48
2:B:159:LEU:HD22	2:B:208:ASN:HB3	1.95	0.48
2:B:396:ASN:HB3	2:D:385:ARG:HA	1.95	0.48
1:A:352:ASP:O	1:A:353:LEU:C	2.52	0.47
1:C:22:LYS:HD2	2:D:34:GLN:HG3	1.94	0.47
1:A:141:TYR:CE1	1:A:157:CYS:HB2	2.49	0.47
2:B:214:GLU:OE2	2:B:290:THR:HB	2.14	0.47
1:A:244:PRO:HA	1:A:337:ASP:OD1	2.14	0.47
1:C:330:HIS:HE1	1:C:332:ALA:HB3	1.78	0.47
1:A:135:HIS:C	1:A:135:HIS:ND1	2.67	0.47
1:A:246:PRO:HD3	1:A:255:TRP:CD1	2.50	0.47
1:A:137:ARG:HG3	1:A:139:TYR:CZ	2.50	0.47
2:D:385:ARG:HG3	2:D:386:TYR:N	2.24	0.47
1:A:54:LEU:HD23	1:A:55:LEU:N	2.29	0.47
1:C:330:HIS:CE1	1:C:332:ALA:HB3	2.50	0.47
1:C:315:ARG:HD2	1:C:340:LEU:O	2.14	0.47
1:C:35:HIS:O	1:C:68:ARG:NH2	2.48	0.47
2:D:18:ARG:HD2	2:D:164:LEU:HB2	1.97	0.47
2:D:259:THR:OG1	2:D:261:GLU:HG3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:LYS:NZ	2:B:336:ASP:OD2	2.48	0.47
2:B:383:PRO:HB2	2:D:400:ASP:OD2	2.15	0.47
1:C:219:PHE:CE2	1:C:240:ARG:HG3	2.50	0.47
2:B:313:TYR:HA	2:B:335:THR:O	2.14	0.47
1:A:372:LEU:HD13	1:A:387:TRP:HB2	1.97	0.46
1:A:298:PHE:CE1	1:A:323:GLU:HB3	2.50	0.46
1:A:206:ARG:CZ	1:A:206:ARG:HB2	2.45	0.46
1:A:34:LEU:O	1:A:35:HIS:C	2.51	0.46
2:B:137:PHE:CD1	2:B:191:PRO:HG3	2.51	0.46
1:C:28:LEU:CD2	3:C:425:SF4:S2	3.02	0.46
2:D:354:LEU:HD23	2:D:371:ALA:HB3	1.97	0.46
2:D:393:GLU:HA	2:D:396:ASN:HD22	1.80	0.46
1:A:139:TYR:N	1:A:139:TYR:CD2	2.84	0.46
1:A:27:GLY:HA3	1:A:148:THR:HG22	1.97	0.46
1:A:322:THR:HG21	1:A:363:ILE:CG2	2.40	0.46
1:A:370:CYS:O	1:A:387:TRP:HA	2.15	0.46
1:C:303:SER:O	1:C:304:GLN:HB2	2.15	0.46
1:A:326:THR:OG1	1:A:327:PRO:HD2	2.16	0.46
1:A:381:LYS:HD3	1:A:381:LYS:HA	1.69	0.46
2:B:175:VAL:CG2	2:B:390:MET:HE3	2.45	0.46
1:A:86:HIS:HE1	1:A:124:ALA:HB2	1.81	0.46
1:C:252:THR:OG1	1:C:398:PHE:HA	2.16	0.46
1:A:27:GLY:CA	1:A:148:THR:HG22	2.47	0.45
2:B:264:LEU:CD2	2:B:267:PRO:HD3	2.47	0.45
1:C:139:TYR:N	1:C:139:TYR:CD2	2.84	0.45
2:B:283:VAL:O	2:B:308:VAL:HG12	2.16	0.45
2:B:385:ARG:HH12	2:D:387:ALA:CB	2.29	0.45
2:B:204:GLN:HB3	2:B:204:GLN:HE21	1.57	0.45
2:D:157:ASN:ND2	2:D:188:VAL:HG13	2.32	0.45
1:A:252:THR:HG23	1:A:398:PHE:CD2	2.51	0.45
1:A:25:PHE:O	1:A:150:PHE:N	2.44	0.45
1:C:372:LEU:HD22	1:C:389:ILE:HD13	1.99	0.45
2:D:356:THR:HG22	2:D:357:GLN:N	2.32	0.45
1:C:24:VAL:O	2:D:35:GLY:HA2	2.17	0.45
2:B:162:THR:H	2:B:168:HIS:CD2	2.17	0.45
2:B:18:ARG:CG	2:B:163:ALA:O	2.64	0.45
1:C:253:THR:OG1	1:C:278:ARG:HD3	2.15	0.45
1:C:71:THR:OG1	1:C:73:VAL:HG12	2.17	0.45
1:A:360:HIS:CE1	1:A:368:THR:HG21	2.52	0.45
2:B:104:PRO:O	2:B:108:SER:HB3	2.16	0.45
2:D:142:ARG:HA	2:D:222:HIS:NE2	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:TRP:O	2:B:272:SER:HB3	2.17	0.44
2:B:283:VAL:HA	2:B:352:LEU:O	2.16	0.44
2:D:66:GLY:O	2:D:68:ASP:N	2.51	0.44
1:A:172:GLU:HB3	1:A:198:PRO:O	2.17	0.44
1:A:304:GLN:N	1:A:306:GLU:OE1	2.49	0.44
2:B:402:TRP:O	2:B:405:PRO:HD2	2.16	0.44
1:C:248:GLY:HA3	1:C:312:PHE:CD1	2.52	0.44
1:C:33:TRP:HD1	1:C:34:LEU:N	2.10	0.44
2:B:123:PRO:HG2	2:B:127:ARG:CG	2.47	0.44
1:A:267:ALA:O	1:A:271:GLU:HG2	2.18	0.44
1:A:32:VAL:O	1:A:62:MET:HE1	2.17	0.44
2:B:273:VAL:HG23	1:C:379:GLU:HG3	2.00	0.44
2:B:408:MET:HE2	2:B:408:MET:HA	2.00	0.44
2:B:48:ARG:HE	2:B:48:ARG:HB2	1.66	0.44
1:C:386:LYS:HD3	1:C:387:TRP:N	2.32	0.44
2:D:208:ASN:O	2:D:231:PHE:HA	2.18	0.44
1:A:290:GLU:HG2	1:A:290:GLU:H	1.68	0.44
2:B:168:HIS:O	2:B:169:ARG:C	2.56	0.44
2:B:264:LEU:HD22	2:B:267:PRO:CD	2.48	0.44
1:C:247:PHE:CZ	1:C:397:HIS:NE2	2.85	0.44
2:D:150:ARG:NH1	2:D:203:GLY:O	2.49	0.44
1:A:24:VAL:O	2:B:35:GLY:HA2	2.18	0.44
2:D:156:CYS:HB3	2:D:207:PHE:CE2	2.53	0.44
1:A:379:GLU:OE2	1:A:385:THR:N	2.51	0.43
1:C:85:ALA:O	1:C:88:GLU:HB3	2.18	0.43
1:A:132:HIS:HB3	1:A:136:VAL:HG13	2.00	0.43
1:C:149:THR:H	1:C:152:GLN:NE2	2.16	0.43
1:A:25:PHE:CZ	2:B:41:LEU:HD21	2.52	0.43
1:C:295:LYS:HA	1:C:366:ASP:OD2	2.18	0.43
1:C:33:TRP:CH2	1:C:151:THR:HA	2.53	0.43
2:D:18:ARG:HD2	2:D:164:LEU:CB	2.48	0.43
2:D:161:ALA:HA	2:D:168:HIS:CD2	2.53	0.43
1:A:232:ALA:HA	1:A:235:ARG:NH1	2.33	0.43
2:B:202:LEU:HD22	2:B:223:LEU:HD11	1.99	0.43
2:B:353:ILE:O	2:B:370:CYS:HA	2.18	0.43
1:A:252:THR:O	1:A:256:LEU:HD22	2.18	0.43
2:B:23:MET:HB3	2:B:23:MET:HE2	1.86	0.43
2:B:357:GLN:HE22	2:B:360:ARG:HH12	1.66	0.43
2:D:419:ARG:N	2:D:420:GLU:HA	2.34	0.43
1:A:22:LYS:N	2:B:59:THR:HG21	2.33	0.43
2:D:174:GLU:HG2	2:D:390:MET:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:378:HIS:ND1	2:D:380:GLN:HG2	2.34	0.43
1:A:200:ARG:HG2	1:A:200:ARG:HH11	1.83	0.42
2:B:157:ASN:HD22	2:B:188:VAL:CG2	2.32	0.42
2:B:66:GLY:O	2:B:68:ASP:N	2.52	0.42
2:D:288:ASP:OD2	2:D:288:ASP:C	2.57	0.42
2:D:41:LEU:O	2:D:45:MET:HB2	2.19	0.42
1:A:128:LEU:HD12	1:A:132:HIS:CE1	2.53	0.42
1:C:19:ARG:HG3	1:C:20:GLY:N	2.34	0.42
2:D:66:GLY:C	2:D:68:ASP:N	2.73	0.42
1:C:33:TRP:HH2	1:C:151:THR:HA	1.84	0.42
1:C:17:ARG:NH1	1:C:349:GLU:OE1	2.52	0.42
1:C:397:HIS:HB3	1:C:398:PHE:HD1	1.83	0.42
2:D:157:ASN:HD21	2:D:187:ASN:HD22	1.67	0.42
1:A:179:LEU:O	1:A:180:PRO:C	2.57	0.42
1:A:21:GLN:HA	2:B:59:THR:OG1	2.19	0.42
2:B:238:GLY:CA	2:B:298:ILE:HD11	2.49	0.42
2:B:23:MET:SD	2:B:26:LEU:HD13	2.59	0.42
1:C:391:LEU:HD23	1:C:408:LEU:HD23	2.01	0.42
2:D:266:GLN:HE21	2:D:267:PRO:N	2.16	0.42
2:D:283:VAL:HA	2:D:352:LEU:O	2.18	0.42
2:D:311:GLY:HA2	2:D:321:LEU:HD21	2.00	0.42
2:B:138:ARG:HG3	2:B:218:SER:HB3	2.00	0.42
1:C:179:LEU:HD23	1:C:179:LEU:HA	1.90	0.42
2:B:66:GLY:C	2:B:68:ASP:H	2.22	0.42
2:B:27:GLN:HB2	2:B:89:MET:HG2	2.02	0.42
1:C:304:GLN:HG3	1:C:327:PRO:HG2	2.01	0.42
1:C:22:LYS:HG2	1:C:351:GLN:HG2	2.02	0.42
1:C:387:TRP:HZ3	1:C:389:ILE:HB	1.84	0.42
2:D:162:THR:H	2:D:168:HIS:CD2	2.25	0.42
2:D:308:VAL:HG13	2:D:348:ALA:HB1	2.02	0.42
1:A:168:THR:O	1:A:214:GLY:HA3	2.20	0.41
1:A:386:LYS:O	1:A:386:LYS:HD3	2.20	0.41
2:B:324:ALA:O	2:B:327:GLU:HB2	2.20	0.41
1:C:102:ASP:O	1:C:104:ARG:HG2	2.20	0.41
2:D:356:THR:CG2	2:D:357:GLN:N	2.83	0.41
2:D:356:THR:H	2:D:359:GLU:HB2	1.85	0.41
2:D:47:GLU:O	2:D:48:ARG:HB3	2.19	0.41
1:C:350:GLY:O	1:C:351:GLN:HB3	2.20	0.41
1:C:32:VAL:O	1:C:35:HIS:HD2	2.03	0.41
2:D:404:HIS:HA	2:D:407:VAL:HG12	2.01	0.41
1:C:54:LEU:HD12	2:D:38:TYR:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:GLN:HE21	1:C:152:GLN:HB2	1.65	0.41
1:C:26:CYS:SG	1:C:28:LEU:HB2	2.61	0.41
1:C:93:VAL:HG12	1:C:97:LEU:HD22	2.03	0.41
1:A:386:LYS:HD3	1:A:386:LYS:C	2.40	0.41
1:C:22:LYS:HB2	2:D:59:THR:HG21	2.03	0.41
1:C:372:LEU:HD12	1:C:372:LEU:HA	1.86	0.41
1:A:311:ARG:C	1:A:311:ARG:HD2	2.40	0.41
2:D:223:LEU:HA	2:D:223:LEU:HD23	1.85	0.41
2:D:360:ARG:CG	2:D:360:ARG:HH11	2.15	0.41
1:A:33:TRP:CD1	1:A:34:LEU:N	2.88	0.41
2:B:208:ASN:O	2:B:231:PHE:HA	2.21	0.41
2:B:282:ARG:CZ	2:B:308:VAL:HG21	2.51	0.41
1:C:326:THR:OG1	1:C:327:PRO:HD2	2.20	0.41
1:C:112:CYS:HB2	1:C:113:PRO:CD	2.47	0.41
1:C:77:GLN:HE21	1:C:77:GLN:HB2	1.71	0.41
1:A:173:LEU:CD2	1:A:220:ILE:HG22	2.51	0.41
1:A:158:LEU:O	1:A:162:VAL:HG23	2.21	0.40
2:D:135:GLU:OE1	2:D:135:GLU:HA	2.21	0.40
1:A:105:GLN:HB3	1:A:139:TYR:CE2	2.57	0.40
1:C:381:LYS:HE2	4:C:426:HOH:O	2.21	0.40
2:D:165:GLY:HA3	2:D:168:HIS:CD2	2.56	0.40
1:A:303:SER:O	1:A:304:GLN:HB2	2.21	0.40
1:C:25:PHE:O	1:C:150:PHE:N	2.48	0.40
1:C:313:LEU:O	1:C:317:CYS:HB2	2.21	0.40
2:B:385:ARG:HD2	2:D:385:ARG:HH11	1.86	0.40
1:C:180:PRO:HG2	1:C:395:PRO:HA	2.04	0.40
2:D:224:GLU:O	2:D:228:LYS:HA	2.20	0.40
2:D:33:PRO:HD3	2:D:96:THR:HB	2.03	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	413/436 (95%)	374 (91%)	35 (8%)	4 (1%)	18	50
1	C	412/436 (94%)	369 (90%)	41 (10%)	2 (0%)	32	67
2	B	418/525 (80%)	387 (93%)	29 (7%)	2 (0%)	32	67
2	D	418/525 (80%)	382 (91%)	34 (8%)	2 (0%)	32	67
All	All	1661/1922 (86%)	1512 (91%)	139 (8%)	10 (1%)	28	63

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	PRO
1	A	344	ASN
1	C	182	VAL
2	D	41	LEU
1	A	118	LYS
2	B	67	THR
2	B	68	ASP
2	D	67	THR
1	A	81	GLY
1	C	32	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	329/344 (96%)	286 (87%)	43 (13%)	5	14
1	C	329/344 (96%)	281 (85%)	48 (15%)	3	11
2	B	338/417 (81%)	290 (86%)	48 (14%)	4	11
2	D	338/417 (81%)	291 (86%)	47 (14%)	4	12
All	All	1334/1522 (88%)	1148 (86%)	186 (14%)	4	12

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	10	CYS
1	A	28	LEU
1	A	33	TRP
1	A	35	HIS
1	A	40	ASP
1	A	55	LEU
1	A	71	THR
1	A	74	LEU
1	A	77	GLN
1	A	84	ASP
1	A	96	LEU
1	A	103	ILE
1	A	104	ARG
1	A	114	SER
1	A	118	LYS
1	A	128	LEU
1	A	129	SER
1	A	136	VAL
1	A	138	VAL
1	A	173	LEU
1	A	188	LEU
1	A	199	VAL
1	A	254	LEU
1	A	256	LEU
1	A	269	LYS
1	A	274	THR
1	A	280	ARG
1	A	292	LEU
1	A	306	GLU
1	A	329	LEU
1	A	334	MET
1	A	341	LEU
1	A	343	SER
1	A	368	THR
1	A	372	LEU
1	A	374	LEU
1	A	386	LYS
1	A	393	PHE
1	A	404	ASP
1	A	408	LEU
1	A	414	ARG
1	A	420	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	3	LEU
2	B	7	THR
2	B	18	ARG
2	B	34	GLN
2	B	42	LEU
2	B	47	GLU
2	B	48	ARG
2	B	56	SER
2	B	58	SER
2	B	59	THR
2	B	61	GLU
2	B	72	LEU
2	B	77	LEU
2	B	94	THR
2	B	101	GLN
2	B	105	ASN
2	B	108	SER
2	B	111	LEU
2	B	140	LEU
2	B	146	VAL
2	B	159	LEU
2	B	168	HIS
2	B	176	THR
2	B	181	THR
2	B	185	LYS
2	B	189	CYS
2	B	197	ASP
2	B	204	GLN
2	B	210	LEU
2	B	227	CYS
2	B	235	VAL
2	B	243	ARG
2	B	251	LYS
2	B	264	LEU
2	B	266	GLN
2	B	273	VAL
2	B	282	ARG
2	B	288	ASP
2	B	290	THR
2	B	330	LEU
2	B	333	LEU
2	B	360	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	370	CYS
2	B	377	VAL
2	B	380	GLN
2	B	385	ARG
2	B	418	PHE
2	B	420	GLU
1	C	7	THR
1	C	11	THR
1	C	15	VAL
1	C	17	ARG
1	C	21	GLN
1	C	28	LEU
1	C	33	TRP
1	C	34	LEU
1	C	63	ILE
1	C	73	VAL
1	C	74	LEU
1	C	77	GLN
1	C	82	LEU
1	C	95	LYS
1	C	97	LEU
1	C	98	GLU
1	C	99	ARG
1	C	103	ILE
1	C	106	LEU
1	C	108	LEU
1	C	119	LEU
1	C	121	LEU
1	C	126	GLU
1	C	128	LEU
1	C	138	VAL
1	C	148	THR
1	C	152	GLN
1	C	172	GLU
1	C	173	LEU
1	C	182	VAL
1	C	199	VAL
1	C	201	MET
1	C	206	ARG
1	C	273	VAL
1	C	274	THR
1	C	292	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	329	LEU
1	C	334	MET
1	C	341	LEU
1	C	343	SER
1	C	372	LEU
1	C	378	LEU
1	C	381	LYS
1	C	386	LYS
1	C	389	ILE
1	C	408	LEU
1	C	414	ARG
1	C	419	LEU
2	D	2	LYS
2	D	7	THR
2	D	9	GLU
2	D	18	ARG
2	D	34	GLN
2	D	45	MET
2	D	49	ARG
2	D	52	ARG
2	D	61	GLU
2	D	102	ASP
2	D	103	ASP
2	D	105	ASN
2	D	111	LEU
2	D	113	LEU
2	D	126	SER
2	D	140	LEU
2	D	149	GLU
2	D	154	VAL
2	D	168	HIS
2	D	175	VAL
2	D	177	LYS
2	D	181	THR
2	D	188	VAL
2	D	199	LEU
2	D	214	GLU
2	D	217	GLU
2	D	225	ARG
2	D	227	CYS
2	D	233	LYS
2	D	251	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	258	VAL
2	D	264	LEU
2	D	266	GLN
2	D	270	SER
2	D	272	SER
2	D	288	ASP
2	D	290	THR
2	D	308	VAL
2	D	315	ARG
2	D	333	LEU
2	D	353	ILE
2	D	360	ARG
2	D	378	HIS
2	D	385	ARG
2	D	412	GLU
2	D	417	MET
2	D	420	GLU

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	360	HIS
1	A	376	ASN
2	B	13	HIS
2	B	31	HIS
2	B	157	ASN
2	B	168	HIS
2	B	187	ASN
2	B	204	GLN
2	B	229	GLN
2	B	266	GLN
2	B	378	HIS
2	B	380	GLN
2	B	404	HIS
1	C	21	GLN
1	C	77	GLN
1	C	152	GLN
1	C	360	HIS
1	C	376	ASN
2	D	13	HIS
2	D	27	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	31	HIS
2	D	157	ASN
2	D	168	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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	425	SF4	2	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, 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	415/436 (95%)	-0.17	5 (1%) 79 78	40, 56, 67, 80	1 (0%)
1	C	414/436 (94%)	-0.24	2 (0%) 90 90	40, 56, 67, 80	1 (0%)
2	B	420/525 (80%)	-0.02	11 (2%) 56 52	39, 56, 73, 79	1 (0%)
2	D	420/525 (80%)	-0.09	6 (1%) 75 75	39, 56, 73, 79	0
All	All	1669/1922 (86%)	-0.13	24 (1%) 75 75	39, 56, 72, 80	3 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33	TRP	5.2
2	B	184	ILE	4.0
1	C	33	TRP	3.8
2	D	67	THR	3.7
2	B	154	VAL	3.6
1	A	135	HIS	3.2
2	B	115	VAL	3.0
1	A	7	THR	3.0
2	B	258	VAL	3.0
2	D	258	VAL	2.7
1	A	90	ASP	2.7
2	B	67	THR	2.6
2	B	183	GLY	2.5
1	C	134	PRO	2.5
2	B	149	GLU	2.4
2	B	203	GLY	2.3
2	B	113	LEU	2.2
2	B	197	ASP	2.1
2	D	184	ILE	2.1
2	D	144	LEU	2.1
2	D	75	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	102	ASP	2.0
2	B	111	LEU	2.0
2	D	74	LYS	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, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	SF4	C	425	8/8	0.99	0.10	-2.06	47,49,50,50	0
3	SF4	A	425	8/8	0.99	0.09	-2.45	49,51,51,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.