



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 10:48 pm BST

PDB ID : 3AER
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 : 2.80 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
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

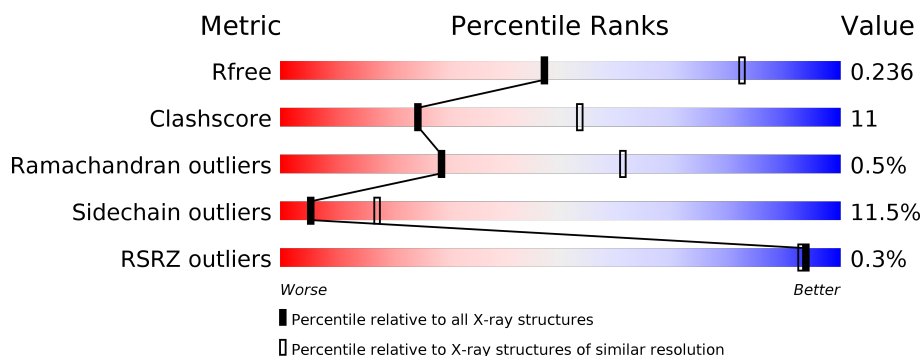
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	436	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 66% 24% 5% 5% </div> </div>
1	C	436	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow, orange, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 72% 20% • 5% </div> </div>
2	B	525	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow, orange, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 58% 18% • 20% </div> </div>
2	D	525	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow, orange, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 62% 15% • 20% </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12974 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
			3174	2016	559	584	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

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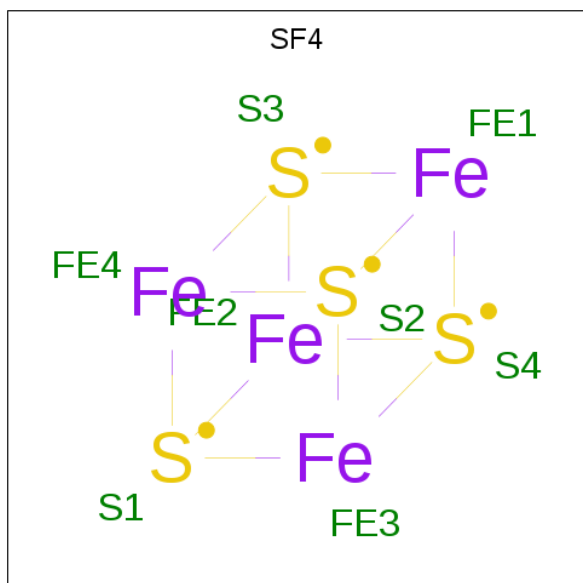
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	ALA	-	EXPRESSION TAG	UNP P26164

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	0	0	0
			3220	2049	557	593	21			
2	D	421	Total	C	N	O	S	0	0	0
			3228	2053	558	596	21			

- 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	34	Total	O	0	0
			34	34		
4	B	43	Total	O	0	0
			43	43		

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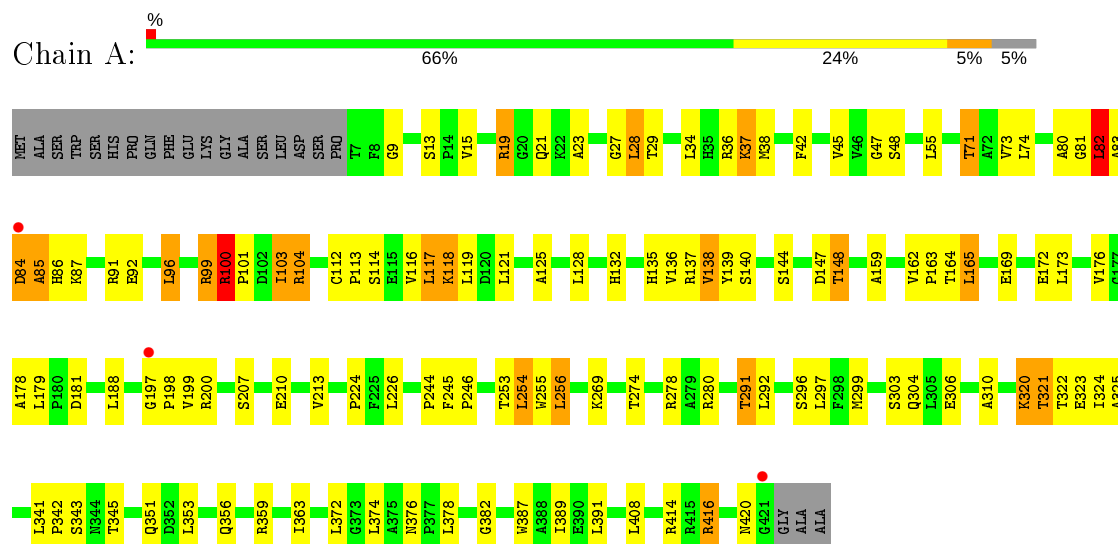
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	41	Total	O	0	0
			41	41		
4	D	54	Total	O	0	0
			54	54		

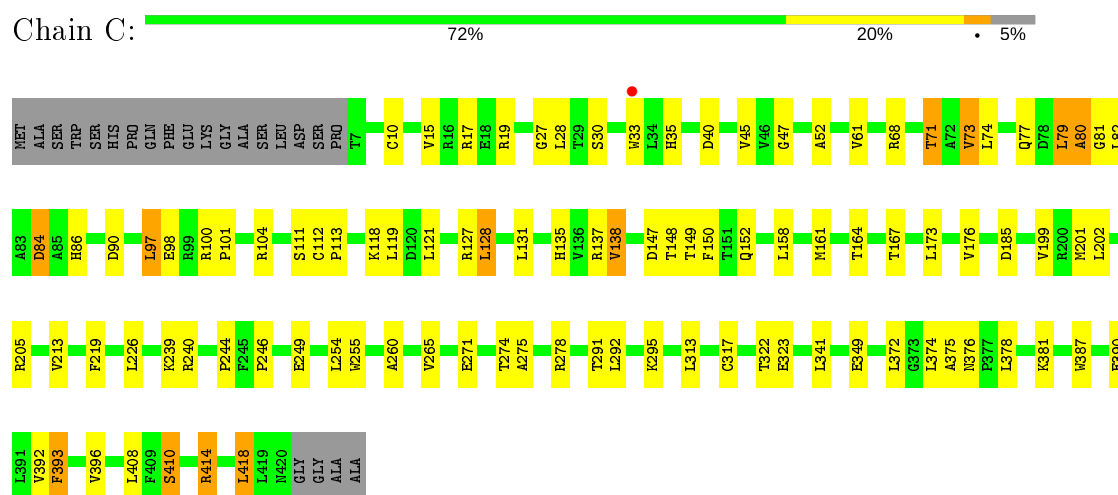
3 Residue-property plots

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 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.42Å 80.94Å 176.73Å 90.00° 100.66° 90.00°	Depositor
Resolution (Å)	47.09 – 2.80 47.09 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.9 (47.09-2.80) 91.9 (47.09-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.187 , 0.237 0.189 , 0.236	Depositor DCC
R_{free} test set	2592 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12974	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.27% 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	0.56	0/3227	0.75	1/4382 (0.0%)
1	C	0.54	1/3239 (0.0%)	0.70	2/4400 (0.0%)
2	B	0.57	0/3291	0.69	1/4479 (0.0%)
2	D	0.56	0/3299	0.70	3/4490 (0.1%)
All	All	0.56	1/13056 (0.0%)	0.71	7/17751 (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	3
1	C	0	1
2	D	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	410	SER	CB-OG	6.14	1.50	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	LEU	CA-CB-CG	7.98	133.66	115.30
2	D	41	LEU	CA-CB-CG	7.43	132.38	115.30
1	C	341	LEU	CA-CB-CG	5.42	127.76	115.30
2	B	18	ARG	NE-CZ-NH1	5.15	122.88	120.30
2	D	264	LEU	CA-CB-CG	5.08	126.98	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	79	LEU	CA-CB-CG	5.07	126.96	115.30
2	D	3	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	GLY	Peptide
1	A	82	LEU	Peptide
1	A	99	ARG	Peptide
1	C	79	LEU	Peptide
2	D	313	TYR	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	88	0
1	C	3174	0	3205	56	0
2	B	3220	0	3245	75	0
2	D	3228	0	3249	82	0
3	A	8	0	0	1	0
3	C	8	0	0	0	0
4	A	34	0	0	2	0
4	B	43	0	0	1	0
4	C	41	0	0	1	0
4	D	54	0	0	1	0
All	All	12974	0	12898	280	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 11.

All (280) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:THR:HG22	1:A:323:GLU:H	1.18	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:LEU:HD21	1:C:387:TRP:CE3	1.94	1.03
2:D:356:THR:HB	2:D:359:GLU:OE2	1.60	1.00
2:D:360:ARG:HG3	2:D:360:ARG:HH11	1.32	0.93
1:A:322:THR:HG22	1:A:323:GLU:N	1.84	0.92
1:C:372:LEU:HD21	1:C:387:TRP:HE3	1.33	0.90
1:A:306:GLU:HG3	1:A:325:ALA:O	1.72	0.89
2:D:353:ILE:HD11	2:D:359:GLU:HB3	1.56	0.88
1:A:83:ALA:HA	1:A:85:ALA:HB3	1.54	0.88
1:A:359:ARG:O	1:A:363:ILE:HD12	1.76	0.84
1:C:372:LEU:O	2:D:44:THR:HG21	1.78	0.83
1:A:376:ASN:HD21	2:D:273:VAL:H	1.24	0.83
2:D:18:ARG:HH11	2:D:18:ARG:HG2	1.42	0.83
1:A:291:THR:HG21	1:A:414:ARG:HH11	1.41	0.83
1:C:80:ALA:CB	1:C:81:GLY:HA2	2.08	0.82
1:C:148:THR:HG23	1:C:152:GLN:HB2	1.59	0.82
2:B:162:THR:H	2:B:168:HIS:HD2	1.26	0.81
1:C:80:ALA:HB3	1:C:81:GLY:HA2	1.63	0.81
1:A:299:MET:CE	1:A:310:ALA:HB2	2.11	0.80
2:D:162:THR:H	2:D:168:HIS:HD2	1.27	0.79
1:A:321:THR:HG21	1:A:345:THR:OG1	1.84	0.78
1:A:42:PHE:HB2	1:A:103:ILE:HG12	1.67	0.76
2:D:345:ILE:O	2:D:348:ALA:O	2.03	0.76
1:A:297:LEU:O	1:A:322:THR:HB	1.88	0.74
1:A:172:GLU:HB2	4:A:453:HOH:O	1.88	0.73
2:B:18:ARG:HD2	2:B:164:LEU:HB2	1.70	0.73
1:A:84:ASP:CB	1:A:87:LYS:H	2.02	0.73
2:B:103:ASP:O	2:B:107:ILE:HG12	1.88	0.72
2:D:377:VAL:HG11	2:D:381:ASP:HB2	1.71	0.70
1:A:100:ARG:H	1:A:101:PRO:CD	2.04	0.70
2:B:273:VAL:H	1:C:376:ASN:HD21	1.41	0.69
1:A:84:ASP:HB3	1:A:87:LYS:H	1.58	0.68
1:C:149:THR:H	1:C:152:GLN:HE21	1.41	0.68
2:B:31:HIS:HD2	2:B:58:SER:OG	1.77	0.68
1:A:27:GLY:HA3	1:A:148:THR:CG2	2.24	0.66
1:A:9:GLY:O	1:A:343:SER:HB3	1.95	0.66
2:D:356:THR:HG22	2:D:358:MET:H	1.60	0.66
1:A:84:ASP:HA	1:A:85:ALA:HB3	1.76	0.65
1:A:299:MET:HE2	1:A:310:ALA:HB2	1.77	0.65
2:B:94:THR:HG22	2:B:96:THR:H	1.60	0.65
1:A:83:ALA:HA	1:A:85:ALA:CB	2.25	0.65
2:D:356:THR:HG22	2:D:357:GLN:N	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:VAL:HB	1:C:71:THR:HB	1.78	0.64
2:D:162:THR:H	2:D:168:HIS:CD2	2.12	0.64
1:A:80:ALA:O	1:A:82:LEU:N	2.31	0.64
2:B:378:HIS:HB3	2:B:380:GLN:OE1	1.96	0.64
1:C:80:ALA:CB	1:C:81:GLY:CA	2.76	0.63
2:B:161:ALA:O	2:B:191:PRO:HD2	1.98	0.62
2:D:360:ARG:HG3	2:D:360:ARG:NH1	2.08	0.62
2:D:175:VAL:HG21	2:D:390:MET:HE1	1.81	0.62
1:A:376:ASN:ND2	2:D:273:VAL:H	1.97	0.62
1:C:372:LEU:HD12	2:D:45:MET:SD	2.39	0.62
2:B:313:TYR:HA	2:B:335:THR:O	1.99	0.61
2:D:285:ILE:HG22	2:D:292:VAL:HG13	1.83	0.61
1:A:125:ALA:HA	1:A:138:VAL:HG22	1.82	0.61
2:B:415:LEU:O	2:B:419:ARG:HG2	2.01	0.61
2:B:61:GLU:OE2	2:B:63:SER:OG	2.12	0.60
2:B:171:ASP:HB3	2:B:390:MET:CE	2.32	0.60
2:D:377:VAL:HG11	2:D:381:ASP:CB	2.31	0.60
1:A:322:THR:HG21	1:A:363:ILE:HG21	1.84	0.60
1:A:45:VAL:HB	1:A:71:THR:HB	1.84	0.60
1:A:27:GLY:HA3	1:A:148:THR:HG21	1.84	0.59
1:A:322:THR:CG2	1:A:323:GLU:N	2.55	0.59
2:B:158:LEU:HB3	2:B:211:MET:CE	2.33	0.59
2:D:45:MET:HE3	2:D:45:MET:HA	1.85	0.59
2:B:171:ASP:HB3	2:B:390:MET:HE2	1.84	0.59
1:C:90:ASP:OD2	1:C:127:ARG:NH1	2.36	0.59
2:B:404:HIS:CE1	2:D:380:GLN:HE22	2.21	0.58
1:C:35:HIS:O	1:C:68:ARG:NH2	2.36	0.58
2:D:356:THR:CG2	2:D:357:GLN:N	2.65	0.58
1:A:162:VAL:HA	1:A:165:LEU:HD22	1.85	0.58
2:D:236:PRO:HG2	2:D:390:MET:HE2	1.86	0.58
2:D:18:ARG:NH1	2:D:18:ARG:HG2	2.14	0.58
2:D:348:ALA:O	2:D:350:PRO:HD3	2.03	0.58
1:C:271:GLU:O	1:C:275:ALA:HB2	2.04	0.57
2:B:380:GLN:H	2:B:380:GLN:CD	2.08	0.57
1:A:45:VAL:HG21	1:A:55:LEU:HD11	1.86	0.57
1:A:306:GLU:CG	1:A:325:ALA:O	2.47	0.57
2:B:162:THR:H	2:B:168:HIS:CD2	2.16	0.57
2:D:380:GLN:HG3	2:D:381:ASP:N	2.19	0.57
2:D:377:VAL:CG1	2:D:381:ASP:HB2	2.35	0.56
1:A:100:ARG:N	1:A:101:PRO:CD	2.68	0.56
2:B:319:ARG:HG3	2:B:320:PRO:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ARG:H	1:A:101:PRO:HD2	1.70	0.56
1:A:84:ASP:HB3	1:A:87:LYS:N	2.19	0.56
2:B:157:ASN:HD22	2:B:188:VAL:H	1.52	0.56
1:A:132:HIS:HB3	1:A:136:VAL:HG13	1.87	0.55
2:B:157:ASN:ND2	2:B:188:VAL:H	2.05	0.55
2:D:312:CYS:SG	2:D:321:LEU:HD22	2.46	0.55
2:D:161:ALA:O	2:D:191:PRO:HD2	2.06	0.55
2:D:52:ARG:HH11	2:D:52:ARG:HG3	1.71	0.54
1:A:84:ASP:HB2	1:A:87:LYS:H	1.72	0.54
2:B:385:ARG:HD2	2:D:385:ARG:NH1	2.22	0.54
1:C:30:SER:HA	1:C:33[B]:TRP:CZ3	2.42	0.54
1:A:224:PRO:HA	1:A:245:PHE:CZ	2.43	0.54
1:A:207:SER:O	1:A:210:GLU:HG2	2.07	0.54
1:C:291:THR:HG21	1:C:414:ARG:HD3	1.89	0.54
1:A:112:CYS:HB2	1:A:113:PRO:HD3	1.88	0.53
1:A:48:SER:HB2	1:A:113:PRO:HG2	1.89	0.53
2:D:289:GLY:H	2:D:314:ASN:HD22	1.55	0.53
2:B:273:VAL:O	2:B:276:THR:HG23	2.08	0.53
1:A:34:LEU:HG	1:A:38:MET:CE	2.38	0.53
1:C:372:LEU:CD2	1:C:387:TRP:HE3	2.15	0.53
2:D:175:VAL:HG21	2:D:390:MET:CE	2.39	0.53
2:B:360:ARG:NH1	2:B:360:ARG:HG3	2.24	0.53
2:B:158:LEU:HB3	2:B:211:MET:HE1	1.91	0.52
1:C:137:ARG:HH22	1:C:164:THR:HB	1.74	0.52
1:C:27:GLY:HA3	1:C:148:THR:HG21	1.90	0.52
1:C:176:VAL:HG13	1:C:202:LEU:HD23	1.89	0.52
2:D:157:ASN:ND2	2:D:188:VAL:H	2.06	0.52
2:B:365:LYS:HE2	2:D:419:ARG:NH2	2.24	0.52
1:A:117:LEU:O	1:A:119:LEU:N	2.41	0.52
1:A:71:THR:HG23	4:B:564:HOH:O	2.08	0.52
2:D:162:THR:N	2:D:168:HIS:HD2	2.01	0.52
2:B:171:ASP:CG	2:B:390:MET:HG3	2.31	0.51
1:C:27:GLY:HA3	1:C:148:THR:CG2	2.40	0.51
1:C:260:ALA:HB1	1:C:265:VAL:HB	1.92	0.51
2:D:162:THR:HG22	2:D:191:PRO:HG2	1.92	0.51
1:C:149:THR:H	1:C:152:GLN:NE2	2.07	0.51
1:A:387:TRP:CZ3	1:A:389:ILE:HB	2.46	0.51
1:A:322:THR:CG2	1:A:363:ILE:HG21	2.41	0.51
2:B:156:CYS:HB3	2:B:207:PHE:CE2	2.45	0.51
1:C:295:LYS:HE2	4:C:449:HOH:O	2.11	0.51
1:A:351:GLN:HG3	1:A:356:GLN:OE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLY:CA	1:A:148:THR:HG23	2.41	0.50
2:B:357:GLN:HG2	2:B:378:HIS:CE1	2.47	0.50
1:C:376:ASN:HB2	2:D:44:THR:HG23	1.93	0.50
2:B:21:THR:HG22	2:B:49:ARG:NH1	2.26	0.50
2:B:360:ARG:HG3	2:B:360:ARG:HH11	1.76	0.50
1:A:27:GLY:HA3	1:A:148:THR:HG23	1.94	0.49
1:A:84:ASP:HB2	1:A:87:LYS:CB	2.42	0.49
1:A:176:VAL:HG12	1:A:226:LEU:HD13	1.93	0.49
2:B:95:CYS:HB3	2:B:124:SER:OG	2.12	0.49
2:B:385:ARG:HG2	2:D:400:ASP:OD2	2.12	0.49
1:A:291:THR:HG21	1:A:414:ARG:HD3	1.93	0.49
2:B:380:GLN:C	2:B:382:PHE:H	2.15	0.49
2:B:47:GLU:HG2	2:B:382:PHE:CZ	2.48	0.49
2:D:24:LYS:HE3	2:D:195:SER:HB3	1.95	0.49
1:A:322:THR:CG2	1:A:323:GLU:H	1.96	0.49
2:B:286:PHE:O	2:B:355:GLY:HA2	2.12	0.49
1:A:118:LYS:HB3	1:A:118:LYS:NZ	2.27	0.49
1:A:27:GLY:CA	1:A:148:THR:CG2	2.90	0.49
2:B:402:TRP:O	2:B:405:PRO:HD2	2.12	0.49
1:C:52:ALA:HA	1:C:71:THR:HG21	1.94	0.49
2:D:157:ASN:ND2	2:D:187:ASN:HB3	2.28	0.49
1:A:246:PRO:HD3	1:A:255:TRP:CD1	2.47	0.49
1:A:382:GLY:O	1:A:416:ARG:NH2	2.46	0.49
2:B:31:HIS:HE1	2:B:102:ASP:OD1	1.95	0.49
2:B:179:LEU:HD11	2:B:209:VAL:HG21	1.94	0.49
2:D:313:TYR:HA	2:D:335:THR:O	2.12	0.49
1:A:99:ARG:CB	1:A:100:ARG:HB2	2.43	0.49
1:C:33[B]:TRP:HZ3	1:C:150:PHE:CE2	2.30	0.48
2:D:415:LEU:O	2:D:419:ARG:HG3	2.13	0.48
1:C:322:THR:OG1	1:C:323:GLU:N	2.46	0.48
2:D:159:LEU:HD21	2:D:223:LEU:HD12	1.94	0.48
1:A:341:LEU:HD23	1:A:342:PRO:HD2	1.96	0.48
1:A:34:LEU:HG	1:A:38:MET:HE3	1.96	0.48
2:B:384:ALA:HB2	2:D:269:TRP:CD1	2.49	0.48
1:C:219:PHE:CE2	1:C:240:ARG:HG3	2.49	0.48
1:C:104:ARG:HH11	1:C:135:HIS:CD2	2.32	0.47
1:C:393:PHE:CD1	1:C:393:PHE:C	2.87	0.47
1:A:296:SER:HA	1:A:320:LYS:O	2.14	0.47
1:C:80:ALA:HB1	1:C:81:GLY:CA	2.43	0.47
2:D:353:ILE:C	2:D:353:ILE:HD12	2.35	0.47
1:A:244:PRO:CG	1:A:254:LEU:HB3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:VAL:HG12	1:C:392:VAL:O	2.15	0.47
1:A:144:SER:O	1:A:148:THR:HG22	2.14	0.47
1:A:255:TRP:HE3	1:A:256:LEU:HD13	1.79	0.47
2:B:266:GLN:HE21	2:B:267:PRO:N	2.13	0.47
1:A:99:ARG:HB2	1:A:100:ARG:HB2	1.95	0.47
1:A:96:LEU:O	1:A:100:ARG:HB3	2.15	0.47
2:B:12:PRO:HB2	2:B:122:LEU:HB3	1.96	0.46
1:C:112:CYS:HB2	1:C:113:PRO:HD3	1.97	0.46
1:A:137:ARG:HD3	1:A:139:TYR:OH	2.15	0.46
1:A:253:THR:OG1	1:A:278:ARG:HD3	2.15	0.46
2:B:92:ALA:HB2	2:B:120:LEU:HD12	1.97	0.46
2:B:217:GLU:OE2	2:B:221:ARG:NH1	2.48	0.46
2:B:357:GLN:NE2	2:B:378:HIS:HB2	2.31	0.46
2:D:359:GLU:HA	2:D:362:ILE:HD12	1.97	0.46
2:D:353:ILE:HD12	2:D:354:LEU:N	2.30	0.46
2:B:178:LEU:HD13	2:B:246:LEU:HD21	1.97	0.46
1:C:86:HIS:ND1	1:C:127:ARG:NH2	2.63	0.46
2:D:148:MET:HE1	2:D:201:LYS:HA	1.98	0.46
2:B:365:LYS:HE2	2:D:419:ARG:HH21	1.80	0.46
2:B:158:LEU:HB3	2:B:211:MET:HE2	1.97	0.46
2:B:38:TYR:C	2:B:38:TYR:CD2	2.88	0.46
1:C:244:PRO:HG2	1:C:254:LEU:HD23	1.97	0.46
1:C:372:LEU:O	2:D:44:THR:CG2	2.57	0.46
1:A:28:LEU:HD22	3:A:425:SF4:S2	2.56	0.46
2:B:408:MET:O	2:B:412:GLU:HG2	2.16	0.46
2:D:378:HIS:NE2	2:D:380:GLN:HG2	2.30	0.46
1:A:320:LYS:HA	1:A:320:LYS:HD2	1.78	0.45
2:D:157:ASN:HD21	2:D:187:ASN:HD22	1.65	0.45
2:B:360:ARG:HA	2:B:370:CYS:SG	2.56	0.45
2:D:360:ARG:HA	2:D:370:CYS:SG	2.55	0.45
2:D:38:TYR:O	2:D:41:LEU:HB3	2.16	0.45
1:A:303:SER:O	1:A:304:GLN:HB2	2.17	0.45
2:B:115:VAL:HB	2:B:116:PRO:HD2	1.97	0.45
1:C:113:PRO:HG3	2:D:96:THR:HG22	1.98	0.45
2:D:45:MET:CE	2:D:45:MET:HA	2.46	0.45
2:D:158:LEU:HB3	2:D:211:MET:CE	2.46	0.45
2:D:377:VAL:HG22	2:D:378:HIS:N	2.32	0.45
2:D:407:VAL:HG23	2:D:408:MET:CE	2.47	0.45
1:C:414:ARG:O	1:C:418:LEU:HB2	2.17	0.45
2:D:236:PRO:HG2	2:D:390:MET:CE	2.46	0.45
1:A:92:GLU:HG3	2:B:3:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ARG:HD3	4:A:452:HOH:O	2.17	0.44
1:C:17:ARG:HD3	1:C:349:GLU:OE1	2.18	0.44
1:C:84:ASP:OD1	1:C:84:ASP:N	2.50	0.44
2:B:224:GLU:HA	2:B:229:GLN:O	2.18	0.44
1:C:246:PRO:HD3	1:C:255:TRP:CD1	2.52	0.44
2:D:285:ILE:CG2	2:D:292:VAL:HG13	2.46	0.44
1:A:172:GLU:OE2	1:A:200:ARG:NH1	2.51	0.44
2:B:273:VAL:H	1:C:376:ASN:ND2	2.10	0.44
1:C:176:VAL:HG12	1:C:226:LEU:HD13	2.00	0.44
2:D:95:CYS:HB3	2:D:124:SER:OG	2.18	0.44
2:D:322:ARG:HG2	2:D:332:ALA:HB3	1.98	0.44
2:B:223:LEU:HA	2:B:223:LEU:HD23	1.89	0.43
1:C:101:PRO:O	1:C:135:HIS:HE1	2.01	0.43
1:A:376:ASN:HD21	2:D:273:VAL:N	2.04	0.43
1:C:185:ASP:OD1	1:C:205:ARG:NH2	2.51	0.43
1:A:125:ALA:HA	1:A:138:VAL:CG2	2.47	0.43
1:A:19:ARG:O	1:A:19:ARG:HG3	2.18	0.43
2:D:161:ALA:HA	2:D:168:HIS:CD2	2.53	0.43
2:D:167:ARG:HD2	2:D:387:ALA:O	2.18	0.43
2:D:9:GLU:OE2	2:D:130:ASN:HB2	2.19	0.43
1:A:47:GLY:O	1:A:73:VAL:HA	2.18	0.43
1:C:128:LEU:HB3	1:C:138:VAL:HG11	2.00	0.43
2:B:407:VAL:HG23	2:B:408:MET:HE2	2.00	0.43
2:B:171:ASP:HB3	2:B:390:MET:HE3	2.01	0.43
2:B:135:GLU:HA	2:B:135:GLU:OE1	2.19	0.42
1:C:249:GLU:OE2	1:C:278:ARG:HD3	2.18	0.42
1:C:47:GLY:O	1:C:73:VAL:HA	2.18	0.42
2:D:407:VAL:O	2:D:411:GLU:HB2	2.19	0.42
1:A:391:LEU:HD23	1:A:408:LEU:HD23	2.01	0.42
2:B:223:LEU:HB3	2:B:229:GLN:HE21	1.84	0.42
2:D:49:ARG:HD3	4:D:566:HOH:O	2.19	0.42
1:A:101:PRO:O	1:A:135:HIS:HE1	2.02	0.42
1:A:84:ASP:HB3	1:A:86:HIS:N	2.34	0.42
2:B:375:ALA:HB1	2:B:376:PRO:HA	2.01	0.42
2:B:364:LYS:HA	2:B:364:LYS:HD2	1.79	0.42
1:C:111:SER:OG	1:C:113:PRO:HD2	2.20	0.42
1:C:158:LEU:HA	1:C:161:MET:HE3	2.01	0.42
1:A:299:MET:HG3	1:A:324:ILE:HG13	2.01	0.42
2:B:30:LEU:HD12	2:B:57:PHE:CZ	2.55	0.42
2:D:161:ALA:HB2	2:D:211:MET:HE3	2.02	0.42
2:B:33:PRO:HD2	2:B:94:THR:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:LEU:HA	1:C:97:LEU:HD13	1.82	0.41
2:B:404:HIS:HE1	2:D:380:GLN:HE22	1.65	0.41
1:A:23:ALA:HB2	1:A:353:LEU:HD22	2.02	0.41
2:B:311:GLY:HA2	2:B:321:LEU:HD21	2.02	0.41
2:D:30:LEU:O	2:D:57:PHE:HA	2.20	0.41
2:D:415:LEU:HD13	2:D:419:ARG:HH12	1.85	0.41
2:D:412:GLU:O	2:D:416:THR:HG23	2.20	0.41
2:D:84:TYR:O	2:D:85:LYS:C	2.58	0.41
2:B:122:LEU:HD22	2:B:132:GLY:HA2	2.02	0.41
1:A:37:LYS:NZ	1:A:179:LEU:O	2.53	0.41
2:B:335:THR:HG21	2:B:340:GLU:HB3	2.03	0.41
2:D:27:GLN:HB2	2:D:89:MET:HG2	2.02	0.41
2:D:288:ASP:HB3	2:D:291:HIS:H	1.85	0.41
1:A:104:ARG:HG2	1:A:104:ARG:HH11	1.86	0.41
1:A:291:THR:CG2	1:A:414:ARG:HH11	2.23	0.41
1:A:159:ALA:O	1:A:163:PRO:HD3	2.20	0.41
2:B:273:VAL:HG21	1:C:375:ALA:HB1	2.02	0.41
2:B:404:HIS:CE1	2:D:380:GLN:NE2	2.87	0.41
2:D:148:MET:HE3	2:D:148:MET:HB2	1.85	0.41
2:B:190:ALA:HA	2:B:191:PRO:C	2.42	0.40
1:C:313:LEU:O	1:C:317:CYS:HB2	2.21	0.40
2:D:236:PRO:HD2	2:D:390:MET:HE3	2.02	0.40
1:A:116:VAL:O	1:A:118:LYS:HE2	2.21	0.40
2:B:411:GLU:HG3	1:C:61:VAL:HG11	2.03	0.40
1:A:27:GLY:N	1:A:148:THR:CG2	2.84	0.40
1:A:27:GLY:H	1:A:148:THR:CG2	2.33	0.40
2:B:319:ARG:CG	2:B:320:PRO:HD3	2.50	0.40
2:B:288:ASP:O	2:B:292:VAL:HG23	2.21	0.40
1:C:390:GLU:HA	1:C:393:PHE:CE2	2.56	0.40
2:D:360:ARG:CG	2:D:360:ARG:NH1	2.76	0.40
2:B:363:ALA:CB	2:B:370:CYS:HB2	2.52	0.40
2:B:7:THR:O	2:B:7:THR:CG2	2.69	0.40
2:D:378:HIS:CD2	2:D:380:GLN:HG2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	389 (94%)	19 (5%)	5 (1%)	13	39
1	C	413/436 (95%)	393 (95%)	19 (5%)	1 (0%)	47	78
2	B	418/525 (80%)	401 (96%)	15 (4%)	2 (0%)	29	61
2	D	419/525 (80%)	392 (94%)	27 (6%)	0	100	100
All	All	1663/1922 (86%)	1575 (95%)	80 (5%)	8 (0%)	29	61

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	GLY
1	A	100	ARG
1	A	198	PRO
2	B	112	ASN
1	A	85	ALA
2	B	381	ASP
1	C	80	ALA
1	A	178	ALA

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%)	283 (86%)	46 (14%)	3	11
1	C	330/344 (96%)	292 (88%)	38 (12%)	5	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	338/417 (81%)	299 (88%)	39 (12%)	5	17
2	D	339/417 (81%)	309 (91%)	30 (9%)	10	29
All	All	1336/1522 (88%)	1183 (88%)	153 (12%)	5	17

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	15	VAL
1	A	19	ARG
1	A	21	GLN
1	A	28	LEU
1	A	29	THR
1	A	37	LYS
1	A	71	THR
1	A	74	LEU
1	A	82	LEU
1	A	84	ASP
1	A	91	ARG
1	A	96	LEU
1	A	100	ARG
1	A	103	ILE
1	A	104	ARG
1	A	114	SER
1	A	118	LYS
1	A	121	LEU
1	A	128	LEU
1	A	138	VAL
1	A	140	SER
1	A	147	ASP
1	A	148	THR
1	A	164	THR
1	A	165	LEU
1	A	169	GLU
1	A	173	LEU
1	A	181	ASP
1	A	188	LEU
1	A	199	VAL
1	A	213	VAL
1	A	254	LEU
1	A	256	LEU

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Mol	Chain	Res	Type
1	A	269	LYS
1	A	274	THR
1	A	280	ARG
1	A	291	THR
1	A	292	LEU
1	A	320	LYS
1	A	321	THR
1	A	372	LEU
1	A	374	LEU
1	A	378	LEU
1	A	416	ARG
1	A	420	ASN
2	B	3	LEU
2	B	7	THR
2	B	18	ARG
2	B	48	ARG
2	B	49	ARG
2	B	61	GLU
2	B	83	ARG
2	B	101	GLN
2	B	111	LEU
2	B	112	ASN
2	B	124	SER
2	B	140	LEU
2	B	142	ARG
2	B	153	GLU
2	B	168	HIS
2	B	185	LYS
2	B	186	VAL
2	B	188	VAL
2	B	210	LEU
2	B	214	GLU
2	B	225	ARG
2	B	228	LYS
2	B	251	LYS
2	B	263	THR
2	B	266	GLN
2	B	273	VAL
2	B	274	ASP
2	B	308	VAL
2	B	319	ARG
2	B	330	LEU

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Mol	Chain	Res	Type
2	B	333	LEU
2	B	360	ARG
2	B	364	LYS
2	B	380	GLN
2	B	381	ASP
2	B	385	ARG
2	B	417	MET
2	B	418	PHE
2	B	420	GLU
1	C	10	CYS
1	C	15	VAL
1	C	19	ARG
1	C	28	LEU
1	C	40	ASP
1	C	71	THR
1	C	73	VAL
1	C	74	LEU
1	C	77	GLN
1	C	82	LEU
1	C	84	ASP
1	C	97	LEU
1	C	98	GLU
1	C	100	ARG
1	C	118	LYS
1	C	119	LEU
1	C	121	LEU
1	C	128	LEU
1	C	131	LEU
1	C	138	VAL
1	C	147	ASP
1	C	167	THR
1	C	173	LEU
1	C	199	VAL
1	C	201	MET
1	C	213	VAL
1	C	239	LYS
1	C	274	THR
1	C	292	LEU
1	C	374	LEU
1	C	378	LEU
1	C	381	LYS
1	C	393	PHE

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Mol	Chain	Res	Type
1	C	396	VAL
1	C	408	LEU
1	C	410	SER
1	C	414	ARG
1	C	418	LEU
2	D	3	LEU
2	D	18	ARG
2	D	59	THR
2	D	100	LEU
2	D	111	LEU
2	D	113	LEU
2	D	140	LEU
2	D	142	ARG
2	D	159	LEU
2	D	168	HIS
2	D	210	LEU
2	D	218	SER
2	D	228	LYS
2	D	251	LYS
2	D	264	LEU
2	D	266	GLN
2	D	273	VAL
2	D	274	ASP
2	D	288	ASP
2	D	308	VAL
2	D	330	LEU
2	D	353	ILE
2	D	360	ARG
2	D	378	HIS
2	D	380	GLN
2	D	385	ARG
2	D	411	GLU
2	D	417	MET
2	D	419	ARG
2	D	420	GLU

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

Mol	Chain	Res	Type
1	A	21	GLN
1	A	135	HIS
1	A	152	GLN

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Mol	Chain	Res	Type
1	A	216	ASN
1	A	360	HIS
1	A	376	ASN
2	B	31	HIS
2	B	34	GLN
2	B	105	ASN
2	B	157	ASN
2	B	168	HIS
2	B	187	ASN
2	B	204	GLN
2	B	229	GLN
2	B	266	GLN
1	C	135	HIS
1	C	152	GLN
1	C	216	ASN
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	101	GLN
2	D	105	ASN
2	D	157	ASN
2	D	168	HIS
2	D	204	GLN
2	D	229	GLN
2	D	266	GLN
2	D	314	ASN
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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	-	-		
3	SF4	C	425	1,2	0,12,12	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	-	-	0/6/5/5
3	SF4	C	425	1,2	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	425	SF4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	415/436 (95%)	-0.38	3 (0%) 87 84	26, 38, 49, 58	0
1	C	414/436 (94%)	-0.33	1 (0%) 95 94	29, 42, 53, 68	0
2	B	420/525 (80%)	-0.34	0 100 100	28, 38, 51, 74	0
2	D	421/525 (80%)	-0.29	1 (0%) 95 94	30, 42, 52, 68	0
All	All	1670/1922 (86%)	-0.34	5 (0%) 94 93	26, 40, 52, 74	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	421	GLY	3.4
2	D	421	ASP	3.0
1	C	33[A]	TRP	2.5
1	A	197	GLY	2.5
1	A	84	ASP	2.1

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
3	SF4	A	425	8/8	0.99	0.09	22,24,25,26	0
3	SF4	C	425	8/8	0.99	0.08	22,25,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.