Full wwPDB X-ray Structure Validation Report (i)

Dec 13, 2023 – 02:11 am GMT

PDB ID	:	2XSH
Title	:	CRYSTAL STRUCTURE OF P4 VARIANT OF BIPHENYL DIOXYGENASE FROM BURKHOLDERIA XENOVORANS LB400 IN COMPLEX WITH 2,6 DI CHLOROBIPHENYL
Authors	:	Kumar, P.; Bolin, J.T.
Deposited on	:	2010-09-29
Resolution	:	2.29 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

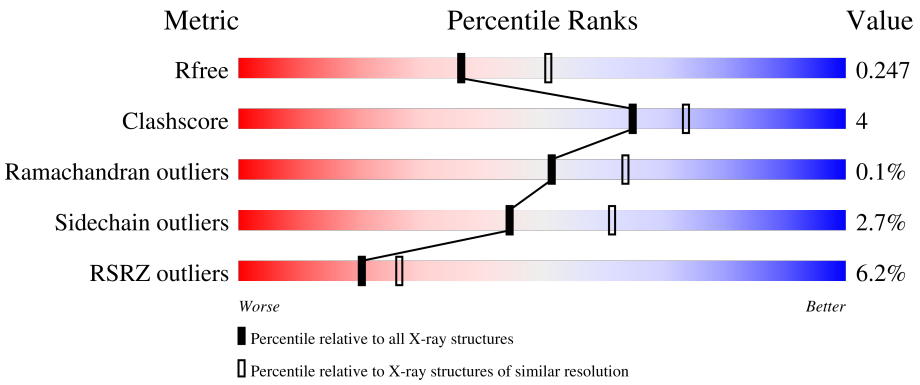
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	459	2%, 86%, 8%, • 6%
1	C	459	3%, 84%, 10%, 6%
1	E	459	3%, 83%, 10%, • 6%
1	G	459	11%, 83%, 10%, 6%
1	I	459	12%, 82%, 12%, 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	459	16% 81% 13% 6%
2	B	188	.% 84% 11%
2	D	188	.% 82% 13%
2	F	188	.% 80% 15%
2	H	188	2% 85% 11%
2	J	188	.% 89% 6%
2	L	188	87% 7%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 30603 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 BIPHENYL DIOXYGENASE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	433	3427	2179	602	622	24	0	0	0
1	C	433	3427	2179	602	622	24	0	0	0
1	E	433	3427	2179	602	622	24	0	0	0
1	G	433	3427	2179	602	622	24	0	0	0
1	I	433	3427	2179	602	622	24	0	0	0
1	K	433	3427	2179	602	622	24	0	0	0

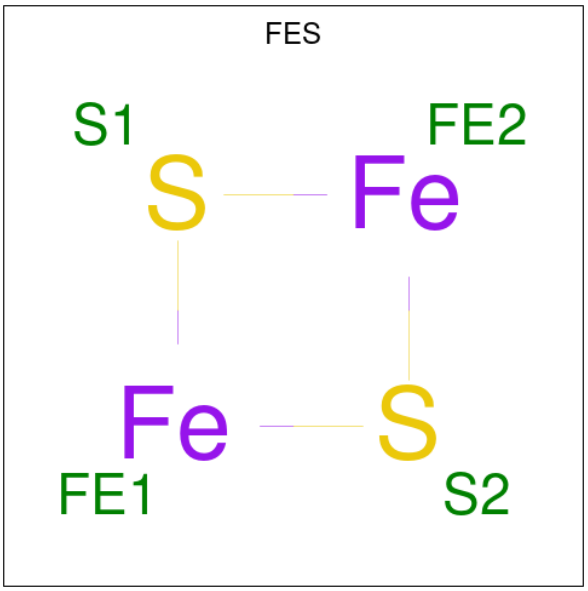
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	ALA	THR	engineered mutation	UNP P37333
C	335	ALA	THR	engineered mutation	UNP P37333
E	335	ALA	THR	engineered mutation	UNP P37333
G	335	ALA	THR	engineered mutation	UNP P37333
I	335	ALA	THR	engineered mutation	UNP P37333
K	335	ALA	THR	engineered mutation	UNP P37333
A	336	MET	PHE	engineered mutation	UNP P37333
C	336	MET	PHE	engineered mutation	UNP P37333
E	336	MET	PHE	engineered mutation	UNP P37333
G	336	MET	PHE	engineered mutation	UNP P37333
I	336	MET	PHE	engineered mutation	UNP P37333
K	336	MET	PHE	engineered mutation	UNP P37333

- Molecule 2 is a protein called BIPHENYL DIOXYGENASE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	180	1496	948	265	279	4	0	0	0
2	D	180	1496	948	265	279	4	0	0	0
2	F	180	1496	948	265	279	4	0	0	0
2	H	180	1496	948	265	279	4	0	0	0
2	J	180	1496	948	265	279	4	0	0	0
2	L	180	1496	948	265	279	4	0	0	0

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

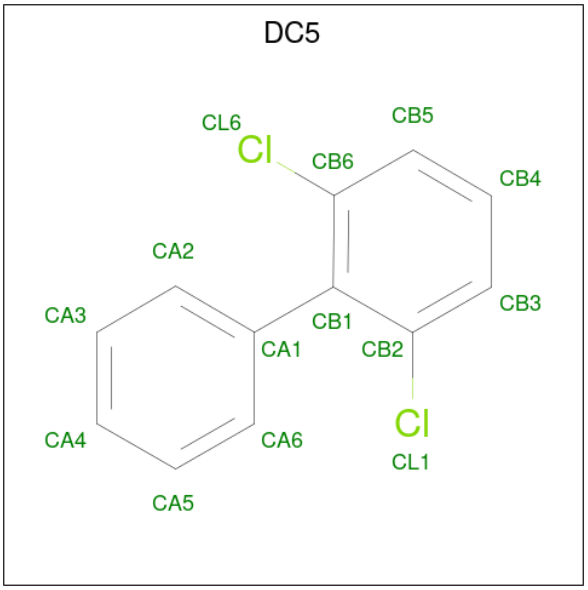


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	A	1	4	2	2	0	0
3	C	1	4	2	2	0	0
3	E	1	4	2	2	0	0
3	G	1	4	2	2	0	0
3	I	1	4	2	2	0	0
3	K	1	4	2	2	0	0

- Molecule 4 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe 1 1	0	0
4	C	1	Total Fe 1 1	0	0
4	E	1	Total Fe 1 1	0	0
4	G	1	Total Fe 1 1	0	0
4	I	1	Total Fe 1 1	0	0
4	K	1	Total Fe 1 1	0	0

- Molecule 5 is 2,6-DICHLOROBIPHENYL (three-letter code: DC5) (formula: $C_{12}H_8Cl_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C Cl 14 12 2	0	0
5	C	1	Total C Cl 14 12 2	0	0
5	E	1	Total C Cl 14 12 2	0	0

- Molecule 6 is water.

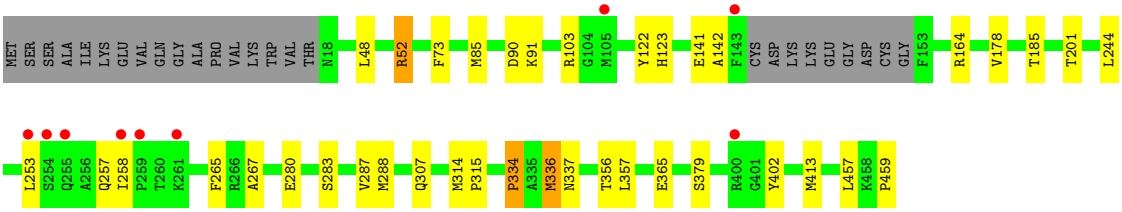
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	139	139	139	0	0
			Total	O		
6	B	82	82	82	0	0
			Total	O		
6	C	129	129	129	0	0
			Total	O		
6	D	81	81	81	0	0
			Total	O		
6	E	128	128	128	0	0
			Total	O		
6	F	79	79	79	0	0
			Total	O		
6	G	82	82	82	0	0
			Total	O		
6	H	51	51	51	0	0
			Total	O		
6	I	80	80	80	0	0
			Total	O		
6	J	32	32	32	0	0
			Total	O		
6	K	79	79	79	0	0
			Total	O		
6	L	31	31	31	0	0

3 Residue-property plots (i)

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

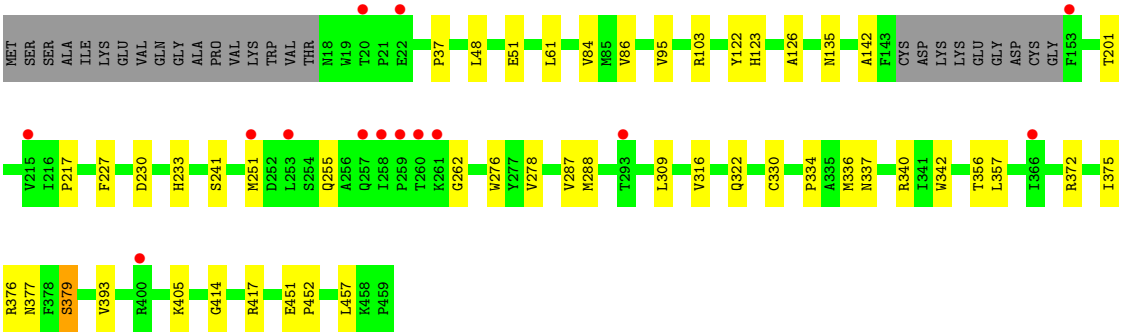
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain A:



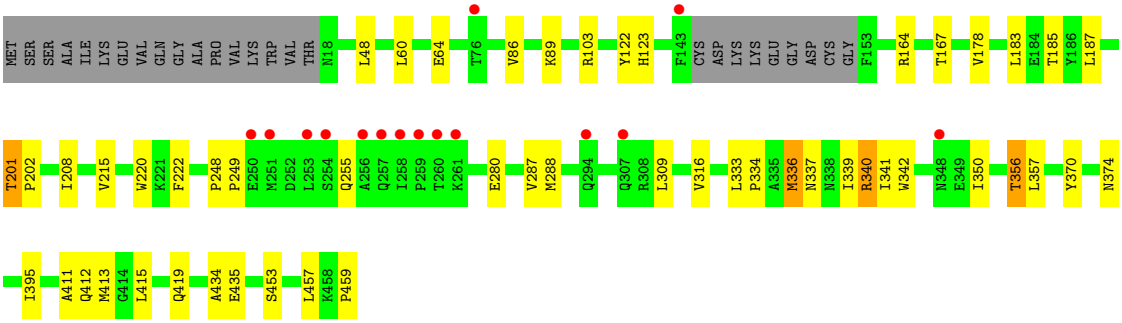
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain C:



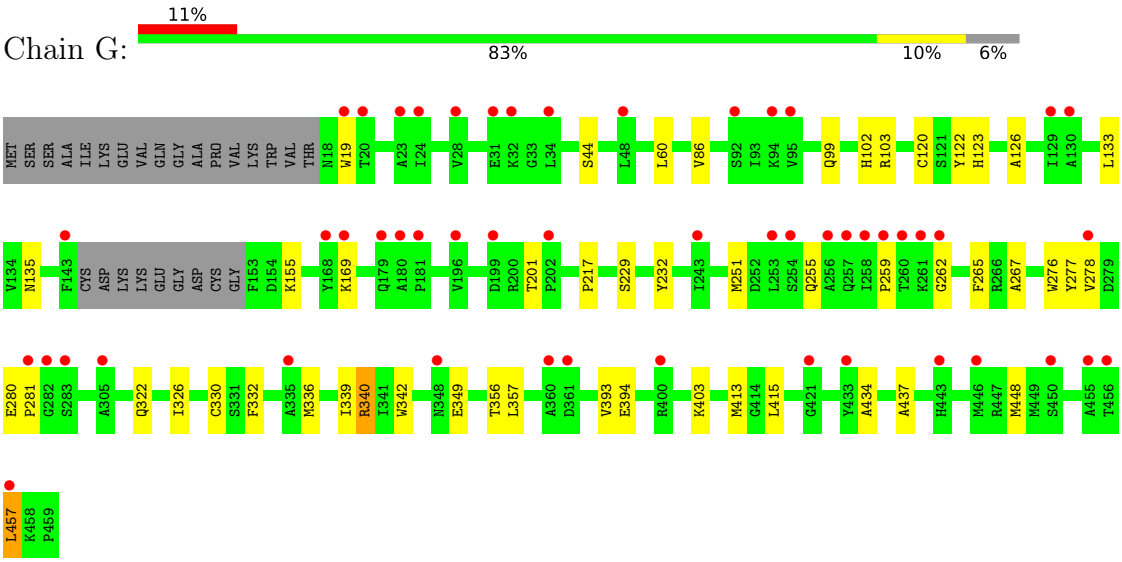
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain E:



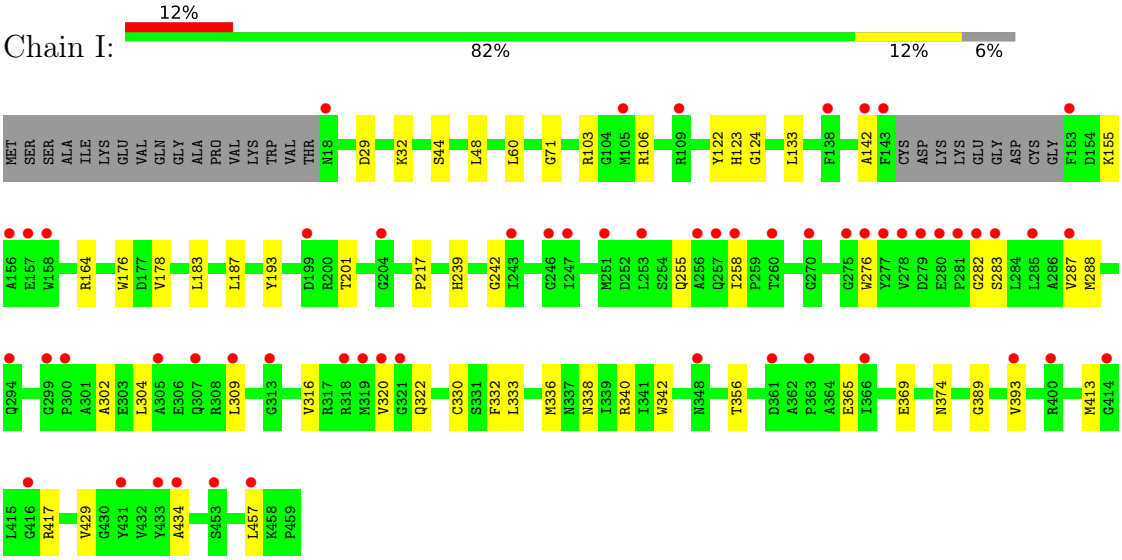
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain G:



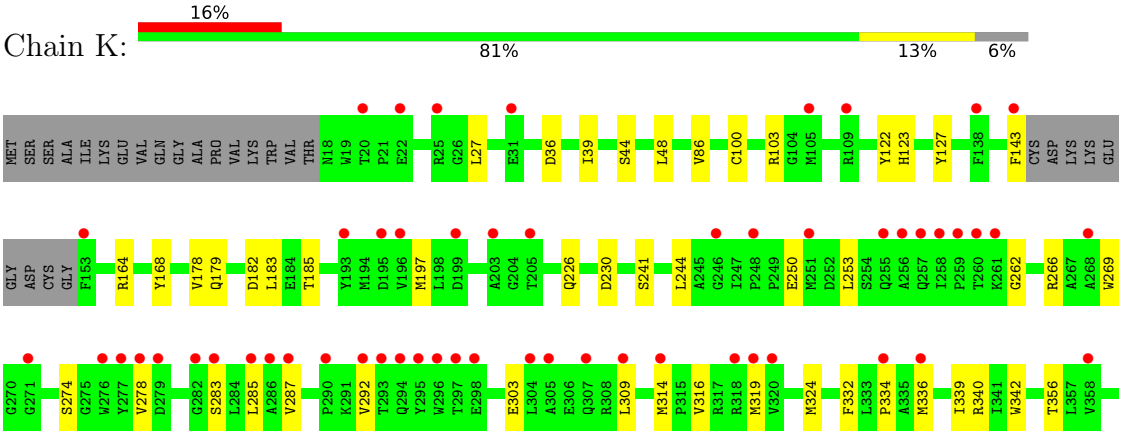
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

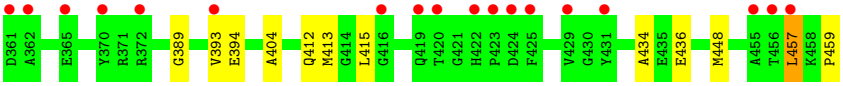
Chain I:



• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

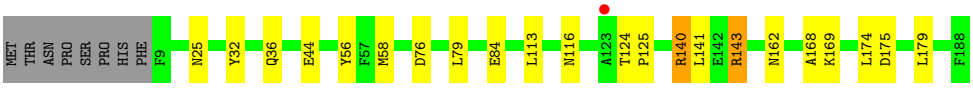
Chain K:





• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain B:

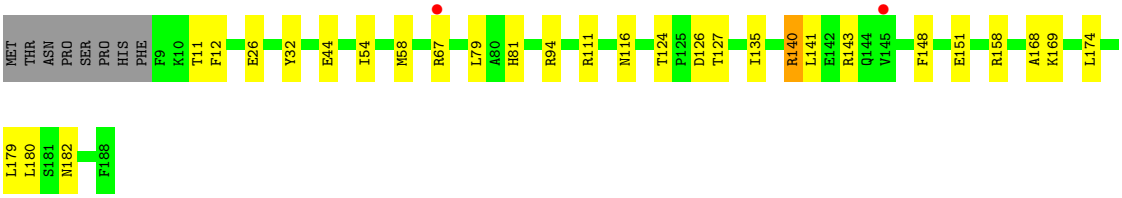


• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain D:

• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain F:

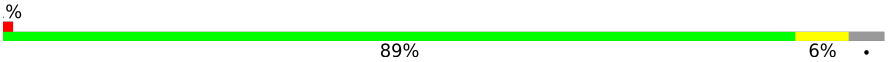


• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain H:

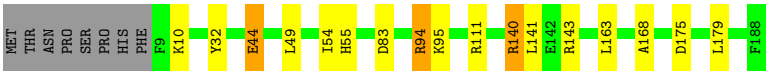
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain J:



• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.73Å 276.76Å 92.32Å 90.00° 117.37° 90.00°	Depositor
Resolution (Å)	138.68 – 2.29 46.47 – 2.29	Depositor EDS
% Data completeness (in resolution range)	87.7 (138.68-2.29) 87.7 (46.47-2.29)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.186 , 0.245 0.188 , 0.247	Depositor DCC
R_{free} test set	7632 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	43.4	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	30603	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FES, FE2, DC5

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	0.50	0/3529	0.61	0/4791
1	C	0.50	0/3529	0.59	0/4791
1	E	0.48	0/3529	0.58	0/4791
1	G	0.39	0/3529	0.52	0/4791
1	I	0.38	0/3529	0.52	0/4791
1	K	0.37	0/3529	0.51	0/4791
2	B	0.51	0/1530	0.64	1/2068 (0.0%)
2	D	0.52	0/1530	0.61	0/2068
2	F	0.50	0/1530	0.62	1/2068 (0.0%)
2	H	0.46	0/1530	0.57	0/2068
2	J	0.43	0/1530	0.57	0/2068
2	L	0.44	0/1530	0.58	0/2068
All	All	0.45	0/30354	0.57	2/41154 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	143	ARG	NE-CZ-NH2	-6.43	117.09	120.30
2	F	143	ARG	NE-CZ-NH2	-5.22	117.69	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3427	0	3276	24	0
1	C	3427	0	3276	28	0
1	E	3427	0	3276	32	0
1	G	3427	0	3276	28	0
1	I	3427	0	3276	34	0
1	K	3427	0	3276	35	0
2	B	1496	0	1447	16	0
2	D	1496	0	1447	26	0
2	F	1496	0	1447	24	0
2	H	1496	0	1447	11	0
2	J	1496	0	1447	6	0
2	L	1496	0	1447	12	0
3	A	4	0	0	1	0
3	C	4	0	0	1	0
3	E	4	0	0	1	0
3	G	4	0	0	1	0
3	I	4	0	0	1	0
3	K	4	0	0	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
5	A	14	0	8	0	0
5	C	14	0	8	0	0
5	E	14	0	8	0	0
6	A	139	0	0	2	0
6	B	82	0	0	2	0
6	C	129	0	0	2	0
6	D	81	0	0	2	0
6	E	128	0	0	0	0
6	F	79	0	0	0	0
6	G	82	0	0	3	0
6	H	51	0	0	0	0
6	I	80	0	0	10	0
6	J	32	0	0	1	0
6	K	79	0	0	5	0
6	L	31	0	0	1	0
All	All	30603	0	28362	238	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 4.

All (238) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:58:MET:HE2	2:D:81:HIS:HB2	1.33	1.06
2:D:58:MET:HE2	2:D:81:HIS:CB	2.01	0.90
1:I:155:LYS:HD2	6:I:2029:HOH:O	1.81	0.81
1:I:133:LEU:HG	6:I:2029:HOH:O	1.83	0.78
1:I:302:ALA:HB3	6:I:2055:HOH:O	1.84	0.77
1:C:201:THR:HB	6:C:2100:HOH:O	1.86	0.75
2:F:58:MET:HE2	2:F:81:HIS:CB	2.18	0.74
2:D:40:HIS:HE1	2:F:151:GLU:OE2	1.71	0.73
1:G:232:TYR:HB2	6:G:2049:HOH:O	1.89	0.73
1:E:123:HIS:HB2	3:E:901:FES:S2	2.29	0.72
2:D:36:GLN:HE21	2:F:12:PHE:H	1.38	0.71
2:D:58:MET:CE	2:D:81:HIS:HB2	2.17	0.71
1:G:123:HIS:HB2	3:G:900:FES:S2	2.30	0.70
2:B:162:ASN:HB3	6:B:2075:HOH:O	1.90	0.70
1:A:287:VAL:HG12	1:A:288:MET:CE	2.22	0.70
1:K:389:GLY:O	1:K:393:VAL:HG23	1.92	0.69
1:I:309:LEU:HD13	1:I:316:VAL:HG11	1.74	0.69
1:A:334:PRO:O	1:A:337:ASN:OD1	2.10	0.68
1:G:339:ILE:HD13	1:G:357:LEU:HG	1.75	0.67
2:D:58:MET:CE	2:D:81:HIS:CB	2.72	0.67
1:K:292:VAL:HA	6:K:2053:HOH:O	1.94	0.66
2:D:41:ARG:HD3	6:D:2019:HOH:O	1.96	0.66
1:A:287:VAL:HG12	1:A:288:MET:HE3	1.78	0.65
1:K:314:MET:HA	6:K:2073:HOH:O	1.96	0.65
1:E:334:PRO:O	1:E:337:ASN:OD1	2.15	0.64
1:K:413:MET:HG2	1:K:434:ALA:HA	1.79	0.64
2:J:76:ASP:HB2	6:J:2016:HOH:O	1.97	0.64
1:C:309:LEU:HD12	1:C:316:VAL:HG11	1.80	0.63
1:A:356:THR:HG23	2:B:79:LEU:HD11	1.81	0.61
1:K:319:MET:HG2	6:K:2048:HOH:O	2.00	0.61
1:I:283:SER:O	1:I:287:VAL:HG23	2.00	0.61
1:A:244:LEU:HD13	1:A:253:LEU:HG	1.82	0.61
2:B:113:LEU:HD21	2:D:113:LEU:HD23	1.82	0.61
2:J:49:LEU:HD21	2:J:163:LEU:HD13	1.84	0.60
1:E:412:GLN:O	1:E:415:LEU:HB2	2.02	0.60
1:K:303:GLU:HA	6:K:2057:HOH:O	2.01	0.59
1:C:262:GLY:HA2	1:C:278:VAL:HG23	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:276:TRP:HB3	1:I:322:GLN:HG3	1.85	0.59
1:K:185:THR:HG22	1:K:459:PRO:HG2	1.84	0.59
1:G:448:MET:HA	1:G:457:LEU:HD11	1.83	0.59
1:K:123:HIS:HB2	3:K:900:FES:S2	2.43	0.59
1:K:309:LEU:HD13	1:K:316:VAL:HG11	1.85	0.58
2:D:40:HIS:CE1	2:F:151:GLU:OE2	2.54	0.58
2:L:44:GLU:HG3	6:L:2011:HOH:O	2.03	0.58
1:C:287:VAL:HG12	1:C:288:MET:CE	2.33	0.58
2:H:32:TYR:CD1	2:J:116:ASN:HA	2.39	0.58
2:B:58:MET:HE1	2:B:174:LEU:HD22	1.85	0.58
2:B:175:ASP:OD2	2:F:111:ARG:HB2	2.04	0.58
1:G:229:SER:HB2	1:G:437:ALA:HB3	1.86	0.57
2:F:168:ALA:O	2:F:169:LYS:HG2	2.04	0.57
2:F:58:MET:HE2	2:F:81:HIS:HB3	1.85	0.57
1:I:123:HIS:HB2	3:I:900:FES:S2	2.43	0.57
2:L:54:ILE:HA	2:L:168:ALA:O	2.06	0.56
1:I:239:HIS:HB3	6:I:2040:HOH:O	2.04	0.56
1:E:287:VAL:HG12	1:E:288:MET:CE	2.36	0.56
1:G:120:CYS:SG	6:G:2023:HOH:O	2.58	0.56
1:I:287:VAL:HG12	1:I:288:MET:HE3	1.87	0.55
2:B:58:MET:CE	2:B:174:LEU:HD22	2.36	0.55
1:K:182:ASP:HB3	6:K:2031:HOH:O	2.06	0.55
2:H:56:TYR:HB3	2:H:84:GLU:HB2	1.89	0.55
1:G:262:GLY:HA2	1:G:278:VAL:HG23	1.89	0.55
1:A:283:SER:O	1:A:287:VAL:HG23	2.06	0.54
1:I:287:VAL:HG12	1:I:288:MET:CE	2.37	0.54
1:G:276:TRP:HB3	1:G:322:GLN:HG3	1.89	0.54
2:D:58:MET:HE1	2:D:184:LEU:HD13	1.90	0.54
1:G:251:MET:HG3	1:G:255:GLN:HB2	1.89	0.54
1:I:201:THR:HG22	1:I:304:LEU:HD23	1.89	0.54
1:E:340:ARG:HD3	1:E:342:TRP:CH2	2.43	0.53
1:K:36:ASP:O	1:K:39:ILE:HG12	2.08	0.53
2:F:58:MET:HE2	2:F:81:HIS:HB2	1.90	0.53
1:G:102:HIS:HB3	6:G:2019:HOH:O	2.09	0.53
2:H:58:MET:HE2	2:H:81:HIS:CB	2.39	0.53
1:C:414:GLY:HA2	1:C:417:ARG:HD2	1.90	0.53
1:E:309:LEU:HD13	1:E:316:VAL:HG11	1.90	0.53
1:I:340:ARG:HD3	1:I:342:TRP:CH2	2.44	0.53
1:G:265:PHE:CZ	1:G:267:ALA:HA	2.43	0.52
1:E:333:LEU:CB	1:E:336:MET:HG3	2.39	0.52
1:G:340:ARG:HD3	1:G:342:TRP:CH2	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:197:MET:HB2	1:K:334:PRO:HB3	1.90	0.52
1:A:413:MET:HG3	1:C:142:ALA:HB1	1.93	0.51
1:G:126:ALA:HB3	1:G:135:ASN:HB3	1.92	0.51
2:D:36:GLN:NE2	2:F:12:PHE:H	2.06	0.51
1:K:266:ARG:NH1	1:K:436:GLU:OE1	2.42	0.51
2:H:70:GLU:H	2:H:70:GLU:CD	2.14	0.51
2:J:73:TYR:CE1	2:J:173:LEU:HD22	2.46	0.51
2:D:32:TYR:CD1	2:F:116:ASN:HA	2.46	0.50
1:K:394:GLU:OE1	2:L:141:LEU:HD13	2.12	0.50
2:D:145:VAL:HG21	2:F:180:LEU:HD11	1.94	0.49
1:A:52:ARG:HD3	6:A:2135:HOH:O	2.11	0.49
1:G:332:PHE:HB3	1:G:339:ILE:HG13	1.94	0.49
1:K:241:SER:HB2	2:L:95:LYS:HG3	1.93	0.49
1:I:183:LEU:O	1:I:187:LEU:HG	2.12	0.49
1:I:44:SER:O	1:I:48:LEU:HD23	2.13	0.49
2:F:58:MET:HE3	2:F:81:HIS:CD2	2.47	0.48
1:I:417:ARG:HH21	1:K:143:PHE:C	2.17	0.48
2:F:124:THR:HB	2:F:127:THR:HB	1.94	0.48
1:A:52:ARG:HD2	6:A:2017:HOH:O	2.14	0.48
1:C:123:HIS:HB2	3:C:900:FES:S2	2.54	0.48
2:L:55:HIS:NE2	2:L:83:ASP:OD2	2.46	0.48
1:I:332:PHE:HB2	6:I:2064:HOH:O	2.13	0.48
1:K:44:SER:O	1:K:48:LEU:HD23	2.14	0.48
1:K:244:LEU:HG	2:L:94:ARG:HG2	1.96	0.48
1:E:287:VAL:HG12	1:E:288:MET:HE3	1.96	0.48
2:B:168:ALA:O	2:B:169:LYS:HG2	2.14	0.47
1:C:287:VAL:HG12	1:C:288:MET:HE2	1.95	0.47
2:F:26:GLU:OE1	2:F:158:ARG:NH2	2.42	0.47
1:A:287:VAL:HG12	1:A:288:MET:HE2	1.96	0.47
1:E:333:LEU:HB3	1:E:336:MET:HG3	1.96	0.47
2:J:111:ARG:HB2	2:L:175:ASP:OD2	2.14	0.47
1:A:142:ALA:HB1	1:E:413:MET:HG3	1.97	0.47
2:L:49:LEU:HD21	2:L:163:LEU:HD13	1.95	0.47
2:L:140:ARG:HG3	2:L:141:LEU:HG	1.96	0.47
1:K:340:ARG:HD3	1:K:342:TRP:CH2	2.50	0.47
1:K:262:GLY:HA2	1:K:278:VAL:HG23	1.97	0.47
1:C:241:SER:HB2	2:D:95:LYS:HG3	1.97	0.46
2:D:67:ARG:NE	2:D:67:ARG:HA	2.31	0.46
1:G:403:LYS:HE3	1:I:176:TRP:HB3	1.98	0.46
1:K:448:MET:HA	1:K:457:LEU:HD11	1.97	0.46
1:I:29:ASP:OD1	1:I:32:LYS:HD2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:VAL:HG12	1:C:288:MET:HE3	1.97	0.46
1:G:413:MET:HG3	1:I:142:ALA:HB1	1.98	0.46
1:E:185:THR:HG22	1:E:459:PRO:HG2	1.98	0.46
1:A:185:THR:HG22	1:A:459:PRO:HG2	1.98	0.46
2:B:25:ASN:HD21	2:D:24:GLN:HG2	1.81	0.46
2:H:122:THR:HG22	2:H:129:GLU:HG3	1.97	0.46
2:H:155:VAL:HB	2:H:169:LYS:HB2	1.98	0.46
1:K:340:ARG:CD	1:K:342:TRP:CH2	2.99	0.45
1:I:71:GLY:HA3	6:I:2013:HOH:O	2.17	0.45
1:E:208:ILE:HD12	1:E:356:THR:OG1	2.15	0.45
1:G:280:GLU:HA	1:G:281:PRO:HD3	1.79	0.45
1:A:265:PHE:CZ	1:A:267:ALA:HA	2.52	0.45
2:B:36:GLN:HE21	2:D:12:PHE:H	1.64	0.45
2:D:140:ARG:HG3	2:D:141:LEU:HG	1.98	0.45
2:F:148:PHE:HB3	2:F:174:LEU:HD11	1.98	0.45
1:I:333:LEU:HD12	1:I:338:ASN:HB3	1.98	0.45
1:I:413:MET:HG2	1:I:434:ALA:HA	1.99	0.45
1:G:217:PRO:HG2	1:G:393:VAL:HG22	1.99	0.45
2:D:36:GLN:HB3	2:F:11:THR:HG23	1.99	0.45
1:E:339:ILE:CD1	1:E:357:LEU:HG	2.47	0.45
1:G:19:TRP:HE1	1:G:44:SER:HB2	1.81	0.45
1:I:123:HIS:N	6:I:2025:HOH:O	2.31	0.44
1:I:193:TYR:CE2	1:I:276:TRP:CH2	3.05	0.44
1:A:90:ASP:O	1:A:91:LYS:HB2	2.18	0.44
1:E:339:ILE:HD13	1:E:357:LEU:HG	1.99	0.44
1:E:411:ALA:HA	1:E:435:GLU:OE2	2.18	0.44
2:F:126:ASP:HB3	2:F:158:ARG:HB2	1.99	0.44
1:K:100:CYS:SG	1:K:127:TYR:OH	2.71	0.44
1:A:123:HIS:HB2	3:A:900:FES:S2	2.58	0.44
1:C:251:MET:HG3	1:C:255:GLN:HB2	1.99	0.44
1:E:287:VAL:HG12	1:E:288:MET:HE2	1.98	0.44
1:E:333:LEU:HB2	1:E:336:MET:HG3	2.00	0.44
1:E:183:LEU:O	1:E:187:LEU:HG	2.18	0.44
1:E:333:LEU:O	1:E:337:ASN:N	2.44	0.44
1:I:124:GLY:N	6:I:2025:HOH:O	2.49	0.44
1:C:227:PHE:CZ	1:C:340:ARG:HD2	2.53	0.44
1:E:356:THR:HG23	2:F:79:LEU:HD11	2.00	0.43
1:G:349:GLU:OE2	2:L:143:ARG:NH2	2.42	0.43
2:H:175:ASP:OD2	2:L:111:ARG:HB2	2.18	0.43
1:I:164:ARG:HD2	1:I:178:VAL:HA	1.99	0.43
2:B:56:TYR:HB3	2:B:84:GLU:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:LEU:HD22	2:D:135:ILE:HD12	2.00	0.43
1:K:283:SER:O	1:K:287:VAL:HG23	2.17	0.43
1:E:164:ARG:HD2	1:E:178:VAL:HA	2.00	0.43
2:J:120:LYS:HB3	2:J:129:GLU:HB2	2.00	0.43
1:G:60:LEU:HD22	1:G:330:CYS:SG	2.59	0.43
1:G:259:PRO:HB2	1:G:277:TYR:CD2	2.54	0.43
1:C:84:VAL:O	1:C:95:VAL:HA	2.18	0.43
2:B:140:ARG:HG3	2:B:141:LEU:HG	2.01	0.43
1:E:222:PHE:CZ	1:E:395:ILE:HG21	2.53	0.43
1:C:37:PRO:HG2	1:C:405:LYS:HA	2.01	0.43
1:C:276:TRP:HB3	1:C:322:GLN:HG3	2.00	0.43
1:E:413:MET:HG2	1:E:434:ALA:HA	1.99	0.43
1:K:332:PHE:HB3	1:K:339:ILE:HA	2.00	0.43
1:A:141:GLU:OE1	1:A:141:GLU:N	2.52	0.43
1:A:365:GLU:H	1:A:365:GLU:CD	2.22	0.43
1:C:372:ARG:HD2	6:C:2105:HOH:O	2.18	0.43
2:D:49:LEU:HD21	2:D:163:LEU:HD13	1.99	0.43
1:G:394:GLU:OE2	1:I:106:ARG:NE	2.52	0.43
1:I:217:PRO:HG2	1:I:393:VAL:HG22	1.99	0.43
1:K:164:ARG:HD2	1:K:178:VAL:HA	2.01	0.43
1:C:376:ARG:NH2	1:C:377:ASN:HD21	2.17	0.42
1:K:412:GLN:O	1:K:415:LEU:HB2	2.19	0.42
1:E:64:GLU:OE1	1:E:167:THR:HG21	2.19	0.42
1:K:168:TYR:HB2	1:K:183:LEU:HD21	2.01	0.42
1:A:314:MET:HA	1:A:315:PRO:HD3	1.90	0.42
1:G:99:GLN:NE2	1:K:404:ALA:HB1	2.35	0.42
1:A:402:TYR:CZ	1:C:51:GLU:HG3	2.54	0.42
1:E:215:VAL:O	2:F:182:ASN:HA	2.20	0.42
1:E:337:ASN:HB3	1:E:357:LEU:O	2.20	0.42
1:K:27:LEU:HD13	1:K:39:ILE:HG22	2.01	0.42
1:I:356:THR:HG21	1:I:374:ASN:HB3	2.00	0.42
1:A:73:PHE:HA	1:A:85:MET:O	2.19	0.42
1:A:164:ARG:HD2	1:A:178:VAL:HA	1.99	0.42
1:I:365:GLU:O	1:I:369:GLU:HG2	2.19	0.42
1:K:244:LEU:HD13	1:K:253:LEU:HG	2.01	0.42
1:K:269:TRP:NE1	1:K:457:LEU:O	2.53	0.42
1:C:375:ILE:O	1:C:379:SER:HB3	2.20	0.42
1:I:60:LEU:HD22	1:I:330:CYS:SG	2.59	0.42
1:I:242:GLY:HA3	6:I:2040:HOH:O	2.19	0.42
1:A:337:ASN:HB3	1:A:357:LEU:O	2.20	0.42
2:D:113:LEU:HD22	2:F:135:ILE:HD12	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:274:SER:HB2	1:K:324:MET:HG3	2.01	0.42
1:C:340:ARG:HD3	1:C:342:TRP:CH2	2.54	0.42
1:G:133:LEU:HG	1:G:155:LYS:HD2	2.01	0.42
2:H:116:ASN:HA	2:L:32:TYR:CD1	2.55	0.42
1:A:379:SER:HB2	6:B:2045:HOH:O	2.20	0.42
1:K:226:GLN:HA	1:K:230:ASP:HB2	2.00	0.42
2:B:113:LEU:CD2	2:D:135:ILE:HD12	2.50	0.41
1:G:356:THR:HG23	2:H:79:LEU:HD11	2.01	0.41
2:B:32:TYR:CG	2:D:116:ASN:HA	2.55	0.41
2:D:99:ASP:OD1	2:F:67:ARG:NE	2.52	0.41
1:C:337:ASN:HB3	1:C:357:LEU:O	2.20	0.41
1:I:429:VAL:HG13	6:I:2045:HOH:O	2.20	0.41
2:B:124:THR:HA	2:B:125:PRO:HD3	1.96	0.41
2:F:54:ILE:HA	2:F:168:ALA:O	2.20	0.41
1:A:336:MET:H	1:A:336:MET:HG2	1.60	0.41
1:C:217:PRO:HG2	1:C:393:VAL:HG22	2.02	0.41
1:C:376:ARG:HD2	6:D:2048:HOH:O	2.21	0.41
2:D:58:MET:HE2	2:D:81:HIS:CG	2.53	0.41
1:E:89:LYS:HE3	1:E:89:LYS:HB2	1.82	0.41
1:E:201:THR:HG22	1:E:202:PRO:HD2	2.03	0.41
2:F:140:ARG:HG3	2:F:141:LEU:HG	2.01	0.41
1:G:413:MET:HG2	1:G:434:ALA:HA	2.02	0.41
2:H:55:HIS:NE2	2:H:83:ASP:OD2	2.39	0.41
1:K:250:GLU:CD	1:K:250:GLU:H	2.24	0.41
1:E:60:LEU:HD23	1:E:341:ILE:HG12	2.02	0.41
1:E:370:TYR:O	1:E:374:ASN:HB2	2.21	0.41
2:H:51:ASP:OD2	2:H:157:ARG:HD2	2.20	0.41
1:C:230:ASP:O	1:C:233:HIS:ND1	2.46	0.41
1:C:334:PRO:O	1:C:337:ASN:OD1	2.39	0.41
1:E:248:PRO:HA	1:E:249:PRO:HD3	1.98	0.41
2:B:116:ASN:HA	2:F:32:TYR:CD1	2.56	0.40
1:C:451:GLU:HA	1:C:452:PRO:HD2	1.93	0.40
1:E:220:TRP:HA	1:E:350:ILE:HG21	2.04	0.40
1:C:61:LEU:HD12	1:C:95:VAL:HG21	2.03	0.40
1:C:126:ALA:HB3	1:C:135:ASN:HB3	2.04	0.40
1:G:326:ILE:HB	1:G:330:CYS:HB3	2.02	0.40
1:I:389:GLY:O	1:I:393:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/459 (94%)	409 (95%)	20 (5%)	0	100	100
1	C	429/459 (94%)	411 (96%)	18 (4%)	0	100	100
1	E	429/459 (94%)	415 (97%)	14 (3%)	0	100	100
1	G	429/459 (94%)	405 (94%)	23 (5%)	1 (0%)	47	58
1	I	429/459 (94%)	403 (94%)	25 (6%)	1 (0%)	47	58
1	K	429/459 (94%)	401 (94%)	28 (6%)	0	100	100
2	B	178/188 (95%)	171 (96%)	7 (4%)	0	100	100
2	D	178/188 (95%)	172 (97%)	6 (3%)	0	100	100
2	F	178/188 (95%)	172 (97%)	6 (3%)	0	100	100
2	H	178/188 (95%)	174 (98%)	4 (2%)	0	100	100
2	J	178/188 (95%)	171 (96%)	7 (4%)	0	100	100
2	L	178/188 (95%)	173 (97%)	5 (3%)	0	100	100
All	All	3642/3882 (94%)	3477 (96%)	163 (4%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	282	GLY
1	G	169	LYS

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	350/372 (94%)	338 (97%)	12 (3%)	37	51
1	C	350/372 (94%)	341 (97%)	9 (3%)	46	63
1	E	350/372 (94%)	337 (96%)	13 (4%)	34	48
1	G	350/372 (94%)	342 (98%)	8 (2%)	50	67
1	I	350/372 (94%)	343 (98%)	7 (2%)	55	72
1	K	350/372 (94%)	342 (98%)	8 (2%)	50	67
2	B	159/167 (95%)	154 (97%)	5 (3%)	40	55
2	D	159/167 (95%)	153 (96%)	6 (4%)	33	47
2	F	159/167 (95%)	155 (98%)	4 (2%)	47	65
2	H	159/167 (95%)	156 (98%)	3 (2%)	57	73
2	J	159/167 (95%)	156 (98%)	3 (2%)	57	73
2	L	159/167 (95%)	154 (97%)	5 (3%)	40	55
All	All	3054/3234 (94%)	2971 (97%)	83 (3%)	44	61

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	52	ARG
1	A	103	ARG
1	A	122	TYR
1	A	201	THR
1	A	257	GLN
1	A	258	ILE
1	A	280	GLU
1	A	307	GLN
1	A	334	PRO
1	A	336	MET
1	A	457	LEU
2	B	44	GLU
2	B	76	ASP
2	B	140	ARG
2	B	143	ARG
2	B	179	LEU
1	C	48	LEU
1	C	86	VAL
1	C	103	ARG
1	C	122	TYR
1	C	330	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	336	MET
1	C	356	THR
1	C	379	SER
1	C	457	LEU
2	D	44	GLU
2	D	76	ASP
2	D	94	ARG
2	D	113	LEU
2	D	121	GLU
2	D	179	LEU
1	E	48	LEU
1	E	86	VAL
1	E	103	ARG
1	E	122	TYR
1	E	201	THR
1	E	255	GLN
1	E	280	GLU
1	E	336	MET
1	E	340	ARG
1	E	356	THR
1	E	419	GLN
1	E	453	SER
1	E	457	LEU
2	F	44	GLU
2	F	94	ARG
2	F	140	ARG
2	F	179	LEU
1	G	86	VAL
1	G	103	ARG
1	G	122	TYR
1	G	201	THR
1	G	336	MET
1	G	340	ARG
1	G	415	LEU
1	G	457	LEU
2	H	10	LYS
2	H	140	ARG
2	H	179	LEU
1	I	103	ARG
1	I	122	TYR
1	I	255	GLN
1	I	258	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	320	VAL
1	I	336	MET
1	I	457	LEU
2	J	140	ARG
2	J	143	ARG
2	J	179	LEU
1	K	86	VAL
1	K	103	ARG
1	K	122	TYR
1	K	179	GLN
1	K	285	LEU
1	K	336	MET
1	K	356	THR
1	K	457	LEU
2	L	10	LYS
2	L	44	GLU
2	L	94	ARG
2	L	140	ARG
2	L	179	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	GLN
2	B	25	ASN
2	B	36	GLN
1	C	377	ASN
1	C	428	ASN
2	D	25	ASN
2	D	36	GLN
2	D	40	HIS
2	D	131	ASN
1	G	373	HIS
2	H	81	HIS
2	H	86	HIS
1	I	419	GLN
1	K	294	GLN
1	K	307	GLN
2	L	81	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 for Mogul analysis.

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	FES	G	900	6,1	0,4,4	-	-	-		
5	DC5	A	902	-	14,15,15	1.25	1 (7%)	16,20,20	1.15	1 (6%)
3	FES	E	901	1	0,4,4	-	-	-		
3	FES	K	900	1	0,4,4	-	-	-		
5	DC5	E	900	-	14,15,15	1.12	0	16,20,20	1.01	1 (6%)
3	FES	A	900	1	0,4,4	-	-	-		
5	DC5	C	902	-	14,15,15	1.07	0	16,20,20	1.14	1 (6%)
3	FES	C	900	1	0,4,4	-	-	-		
3	FES	I	900	1	0,4,4	-	-	-		

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	FES	G	900	6,1	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DC5	A	902	-	-	0/0/4/4	0/2/2/2
3	FES	E	901	1	-	-	0/1/1/1
5	DC5	E	900	-	-	0/0/4/4	0/2/2/2
3	FES	K	900	1	-	-	0/1/1/1
3	FES	A	900	1	-	-	0/1/1/1
5	DC5	C	902	-	-	0/0/4/4	0/2/2/2
3	FES	C	900	1	-	-	0/1/1/1
3	FES	I	900	1	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	902	DC5	CB2-CB1	-2.17	1.39	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	902	DC5	CB2-CB1-CB6	-3.74	116.83	125.49
5	A	902	DC5	CB2-CB1-CB6	-3.70	116.93	125.49
5	E	900	DC5	CB2-CB1-CB6	-3.14	118.22	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	900	FES	1	0
3	E	901	FES	1	0
3	K	900	FES	1	0
3	A	900	FES	1	0
3	C	900	FES	1	0
3	I	900	FES	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	433/459 (94%)	-0.35	9 (2%) 63 70	24, 38, 56, 70	18 (4%)
1	C	433/459 (94%)	-0.17	14 (3%) 47 54	27, 41, 61, 76	18 (4%)
1	E	433/459 (94%)	-0.14	15 (3%) 44 51	24, 43, 68, 78	18 (4%)
1	G	433/459 (94%)	0.62	51 (11%) 4 6	43, 82, 116, 130	18 (4%)
1	I	433/459 (94%)	0.74	57 (13%) 3 4	39, 84, 136, 162	18 (4%)
1	K	433/459 (94%)	0.91	73 (16%) 1 2	42, 87, 151, 175	18 (4%)
2	B	180/188 (95%)	-0.32	1 (0%) 89 92	26, 36, 57, 65	4 (2%)
2	D	180/188 (95%)	-0.15	2 (1%) 80 85	28, 40, 58, 62	4 (2%)
2	F	180/188 (95%)	-0.34	2 (1%) 80 85	26, 38, 56, 62	4 (2%)
2	H	180/188 (95%)	-0.26	3 (1%) 70 76	34, 49, 67, 79	4 (2%)
2	J	180/188 (95%)	-0.11	1 (0%) 89 92	35, 56, 76, 83	4 (2%)
2	L	180/188 (95%)	-0.07	0 100 100	34, 53, 76, 87	4 (2%)
All	All	3678/3882 (94%)	0.13	228 (6%) 20 26	24, 51, 113, 175	132 (3%)

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	258	ILE	15.6
1	G	257	GLN	9.6
1	K	282	GLY	8.8
1	G	258	ILE	8.0
1	I	282	GLY	7.9
1	G	260	THR	7.6
1	K	290	PRO	7.0
1	I	278	VAL	6.8
1	K	248	PRO	6.0
1	K	257	GLN	6.0
1	K	292	VAL	5.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	258	ILE	5.9
1	K	320	VAL	5.8
1	G	254	SER	5.8
1	K	22	GLU	5.7
1	I	281	PRO	5.7
1	C	258	ILE	5.6
1	G	259	PRO	5.6
1	K	294	GLN	5.6
1	I	143	PHE	5.6
1	K	455	ALA	5.5
1	K	361	ASP	5.3
1	K	278	VAL	5.3
1	I	366	ILE	5.1
1	K	277	TYR	5.1
1	I	258	ILE	5.1
1	G	253	LEU	5.0
1	K	420	THR	5.0
1	K	370	TYR	4.8
1	G	261	LYS	4.8
1	K	424	ASP	4.7
1	K	314	MET	4.7
1	I	199	ASP	4.6
1	K	295	TYR	4.6
1	G	256	ALA	4.6
1	K	305	ALA	4.6
1	I	142	ALA	4.5
1	K	260	THR	4.4
1	I	305	ALA	4.4
1	G	202	PRO	4.4
1	K	153	PHE	4.3
1	E	260	THR	4.2
1	I	277	TYR	4.1
1	I	280	GLU	4.0
1	K	319	MET	3.9
1	C	257	GLN	3.8
1	K	256	ALA	3.8
1	I	279	ASP	3.8
1	I	270	GLY	3.7
1	K	196	VAL	3.7
1	K	143	PHE	3.6
1	G	92	SER	3.6
1	A	254	SER	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	246	GLY	3.6
1	A	143	PHE	3.5
1	I	276	TRP	3.5
1	K	422	HIS	3.5
1	K	203	ALA	3.5
1	I	285	LEU	3.4
1	G	196	VAL	3.4
1	K	138	PHE	3.4
1	K	276	TRP	3.4
1	K	251	MET	3.4
1	I	253	LEU	3.3
1	K	318	ARG	3.3
1	K	307	GLN	3.3
1	E	250	GLU	3.3
1	K	362	ALA	3.2
1	E	256	ALA	3.2
1	G	305	ALA	3.2
1	I	300	PRO	3.2
1	I	416	GLY	3.2
1	C	22	GLU	3.1
1	G	180	ALA	3.1
1	K	372	ARG	3.1
1	G	169	LYS	3.1
1	I	457	LEU	3.1
1	G	34	LEU	3.1
1	E	253	LEU	3.1
1	G	48	LEU	3.1
1	G	282	GLY	3.1
1	G	199	ASP	3.0
1	K	457	LEU	3.0
1	K	259	PRO	3.0
1	G	457	LEU	3.0
1	I	361	ASP	3.0
1	I	156	ALA	3.0
1	K	285	LEU	3.0
1	K	199	ASP	3.0
1	K	283	SER	2.9
1	K	423	PRO	2.9
1	I	287	VAL	2.9
1	I	294	GLN	2.9
1	K	431	TYR	2.9
1	C	261	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	129	ILE	2.8
1	K	261	LYS	2.8
1	I	307	GLN	2.8
1	G	433	TYR	2.8
1	I	414	GLY	2.8
1	K	429	VAL	2.8
1	G	283	SER	2.8
1	I	243	ILE	2.8
2	D	145	VAL	2.8
1	G	94	LYS	2.8
1	C	260	THR	2.8
1	K	297	THR	2.8
1	E	261	LYS	2.8
1	G	335	ALA	2.7
1	I	247	ILE	2.7
1	C	259	PRO	2.7
1	K	268	ALA	2.7
1	K	246	GLY	2.7
1	I	153	PHE	2.7
1	I	309	LEU	2.7
1	G	400	ARG	2.7
1	K	296	TRP	2.7
1	G	421	GLY	2.7
1	E	259	PRO	2.7
1	I	453	SER	2.7
1	I	320	VAL	2.7
1	K	20	THR	2.7
1	K	304	LEU	2.7
1	E	257	GLN	2.7
1	I	434	ALA	2.6
1	I	318	ARG	2.6
1	G	143	PHE	2.6
1	E	251	MET	2.6
1	K	205	THR	2.6
1	G	28	VAL	2.6
1	K	309	LEU	2.6
1	G	446	MET	2.6
1	G	243	ILE	2.6
1	I	158	TRP	2.6
1	K	334	PRO	2.6
1	K	336	MET	2.6
1	G	130	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	400	ARG	2.6
1	A	261	LYS	2.6
1	C	366	ILE	2.6
1	I	204	GLY	2.5
1	K	286	ALA	2.5
2	D	16	SER	2.5
1	G	281	PRO	2.5
1	K	255	GLN	2.5
1	I	313	GLY	2.5
1	G	20	THR	2.5
1	G	262	GLY	2.5
1	E	254	SER	2.5
1	G	361	ASP	2.5
1	I	109	ARG	2.5
1	I	321	GLY	2.5
1	I	393	VAL	2.5
1	G	168	TYR	2.5
1	I	251	MET	2.4
1	K	31	GLU	2.4
1	I	256	ALA	2.4
2	H	52	LYS	2.4
1	K	293	THR	2.4
1	K	193	TYR	2.4
1	I	348	ASN	2.4
1	C	251	MET	2.4
1	I	105	MET	2.4
1	K	393	VAL	2.4
1	I	283	SER	2.4
1	E	258	ILE	2.4
1	A	400	ARG	2.4
1	K	416	GLY	2.4
1	G	23	ALA	2.4
1	I	363	PRO	2.4
1	C	153	PHE	2.4
1	G	179	GLN	2.3
1	I	260	THR	2.3
1	K	456	THR	2.3
1	G	348	ASN	2.3
1	G	450	SER	2.3
1	K	419	GLN	2.3
1	I	18	ASN	2.3
1	K	358	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	67	ARG	2.3
1	K	298	GLU	2.3
1	G	19	TRP	2.3
1	E	143	PHE	2.3
1	G	278	VAL	2.3
2	B	123	ALA	2.3
1	C	253	LEU	2.2
1	G	456	THR	2.2
1	I	299	GLY	2.2
1	I	431	TYR	2.2
1	G	24	ILE	2.2
1	G	31	GLU	2.2
1	I	433	TYR	2.2
1	I	319	MET	2.2
1	K	287	VAL	2.2
1	K	271	GLY	2.2
1	A	105	MET	2.2
1	E	348	ASN	2.2
1	I	138	PHE	2.2
1	A	253	LEU	2.2
1	G	443	HIS	2.1
1	K	425	PHE	2.1
1	K	105	MET	2.1
1	G	455	ALA	2.1
2	H	58	MET	2.1
1	E	76	THR	2.1
1	I	157	GLU	2.1
1	K	25	ARG	2.1
1	K	365	GLU	2.1
1	A	259	PRO	2.1
1	G	32	LYS	2.1
1	K	195	ASP	2.1
1	C	293	THR	2.1
1	A	255	GLN	2.1
1	E	307	GLN	2.1
1	C	20	THR	2.1
1	G	181	PRO	2.1
2	F	67	ARG	2.0
1	G	360	ALA	2.0
1	C	215	VAL	2.0
1	K	279	ASP	2.0
2	H	160	ASP	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	294	GLN	2.0
1	I	257	GLN	2.0
1	K	109	ARG	2.0
1	G	95	VAL	2.0
2	F	145	VAL	2.0
1	I	275	GLY	2.0
1	I	400	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DC5	C	902	14/14	0.84	0.24	71,73,74,74	0
5	DC5	A	902	14/14	0.85	0.18	54,58,61,61	0
5	DC5	E	900	14/14	0.85	0.16	72,74,76,76	0
4	FE2	G	901	1/1	0.96	0.11	58,58,58,58	0
3	FES	I	900	4/4	0.97	0.12	62,62,64,66	0
3	FES	K	900	4/4	0.97	0.12	56,57,57,59	0
3	FES	G	900	4/4	0.98	0.11	72,73,73,74	0
3	FES	A	900	4/4	0.99	0.11	38,39,39,40	0
4	FE2	I	901	1/1	0.99	0.09	58,58,58,58	0
4	FE2	K	901	1/1	0.99	0.09	74,74,74,74	0
3	FES	C	900	4/4	0.99	0.10	27,31,32,33	0
3	FES	E	901	4/4	0.99	0.11	36,38,38,40	0
4	FE2	A	901	1/1	0.99	0.14	34,34,34,34	0
4	FE2	C	901	1/1	1.00	0.12	37,37,37,37	0
4	FE2	E	902	1/1	1.00	0.12	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.