Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:28 PM GMT

PDB ID	:	4F0X
Title	:	Crystal structure of human Malonyl-CoA Decarboxylase (Peroxisomal Isoform)
Authors	:	Aparicio, D.; Perez, R.; Fita, I.
Deposited on	:	2012-05-05
Resolution	:	3.29 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

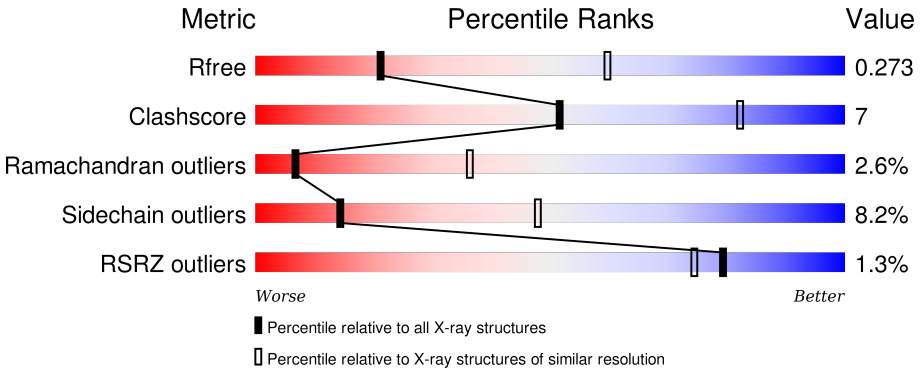
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.29 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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 <=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	458	79% 18%
1	B	458	76% 17%
1	C	458	78% 17%
1	D	458	74% 19% 5%
1	E	458	75% 18%

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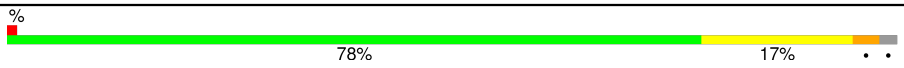
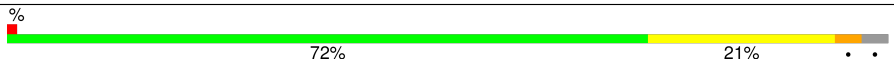
Mol	Chain	Length	Quality of chain
1	F	458	
1	G	458	
1	H	458	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	0OR	B	501[A]	-	-	-	X
2	0OR	D	501[A]	-	-	-	X
2	0OR	E	501[A]	-	-	-	X
2	0OR	G	501[A]	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 28107 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 Malonyl-CoA decarboxylase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3581	2282	633	651	15			
1	B	440	Total	C	N	O	S	0	0	0
			3465	2212	611	627	15			
1	C	446	Total	C	N	O	S	0	0	0
			3503	2235	618	635	15			
1	D	445	Total	C	N	O	S	0	0	0
			3495	2229	616	635	15			
1	E	439	Total	C	N	O	S	0	0	0
			3461	2210	610	626	15			
1	F	449	Total	C	N	O	S	0	0	0
			3525	2249	621	640	15			
1	G	442	Total	C	N	O	S	0	0	0
			3475	2218	613	629	15			
1	H	446	Total	C	N	O	S	0	0	0
			3510	2240	619	636	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	GLY	-	EXPRESSION TAG	UNP O95822
A	37	SER	-	EXPRESSION TAG	UNP O95822
A	38	GLY	-	EXPRESSION TAG	UNP O95822
B	36	GLY	-	EXPRESSION TAG	UNP O95822
B	37	SER	-	EXPRESSION TAG	UNP O95822
B	38	GLY	-	EXPRESSION TAG	UNP O95822
C	36	GLY	-	EXPRESSION TAG	UNP O95822
C	37	SER	-	EXPRESSION TAG	UNP O95822
C	38	GLY	-	EXPRESSION TAG	UNP O95822
D	36	GLY	-	EXPRESSION TAG	UNP O95822
D	37	SER	-	EXPRESSION TAG	UNP O95822
D	38	GLY	-	EXPRESSION TAG	UNP O95822
E	36	GLY	-	EXPRESSION TAG	UNP O95822

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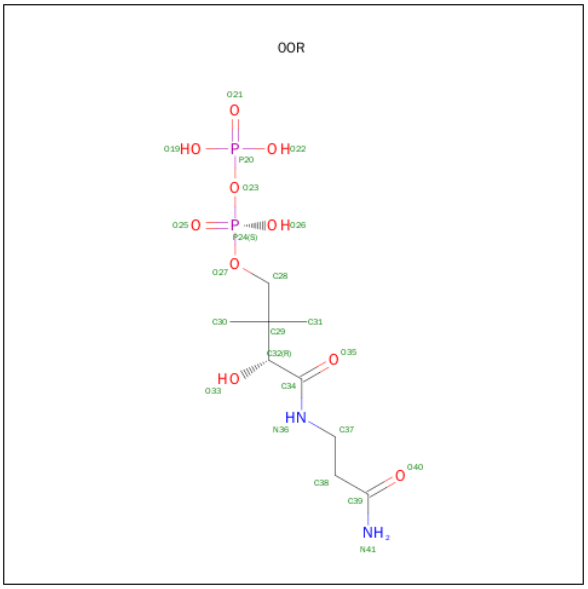
Chain	Residue	Modelled	Actual	Comment	Reference
E	37	SER	-	EXPRESSION TAG	UNP O95822
E	38	GLY	-	EXPRESSION TAG	UNP O95822
F	36	GLY	-	EXPRESSION TAG	UNP O95822
F	37	SER	-	EXPRESSION TAG	UNP O95822
F	38	GLY	-	EXPRESSION TAG	UNP O95822
G	36	GLY	-	EXPRESSION TAG	UNP O95822
G	37	SER	-	EXPRESSION TAG	UNP O95822
G	38	GLY	-	EXPRESSION TAG	UNP O95822
H	36	GLY	-	EXPRESSION TAG	UNP O95822
H	37	SER	-	EXPRESSION TAG	UNP O95822
H	38	GLY	-	EXPRESSION TAG	UNP O95822

- Molecule 2 is N 3 -[(2R)-2-HYDROXY-4-{[(S)-HYDROXY(PHOSPHONOOXY)PHOSPHORYL]OXY}-3,3-DIMETHYLBUTANOYL]-BETA-ALANINAMIDE (three-letter code: 0OR) (formula: $C_9H_{20}N_2O_{10}P_2$).



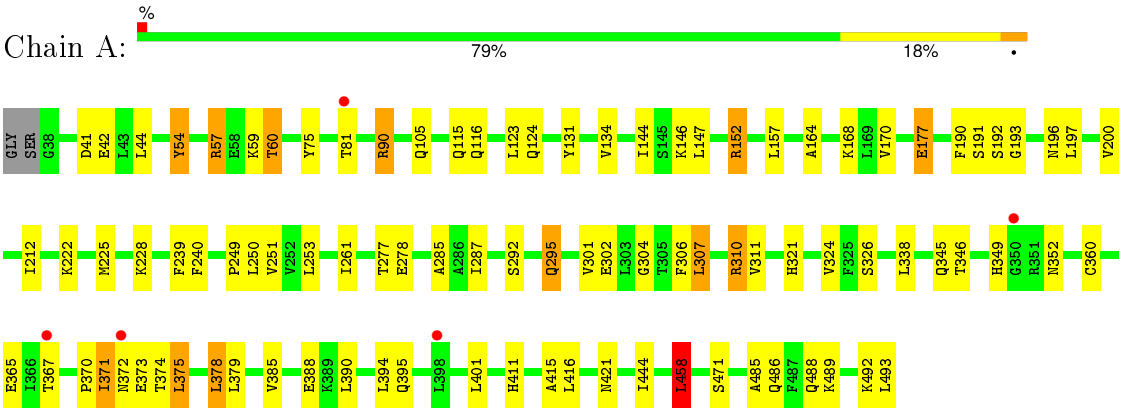
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	1
			23	9	2	10	2		
2	D	1	Total	C	N	O	P	0	1
			23	9	2	10	2		
2	E	1	Total	C	N	O	P	0	1
			23	9	2	10	2		
2	G	1	Total	C	N	O	P	0	1
			23	9	2	10	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

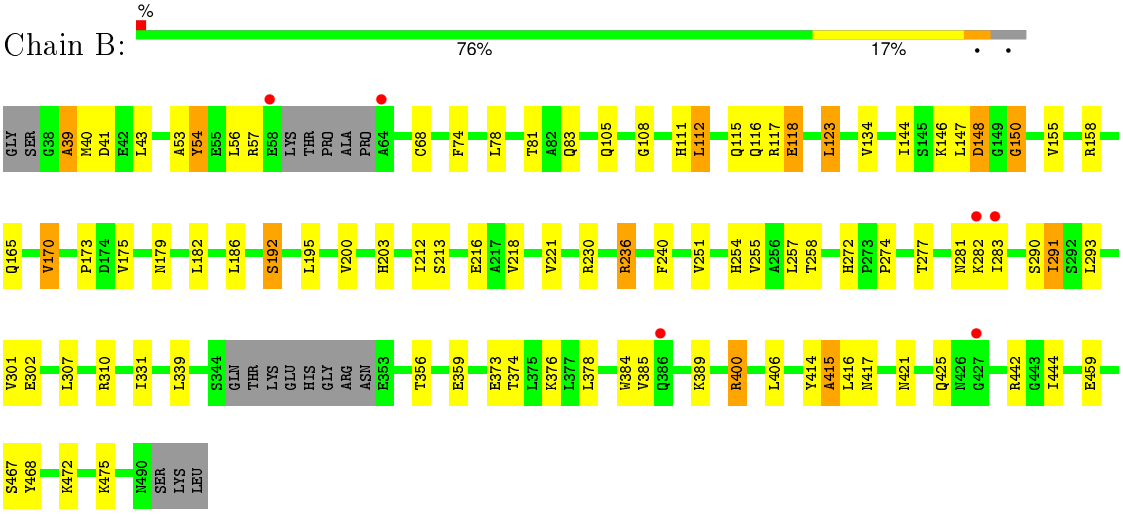
- Molecule 1: Malonyl-CoA decarboxylase, mitochondrial

Chain A:



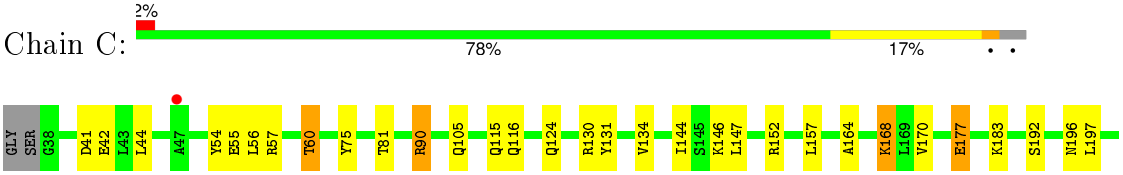
- Molecule 1: Malonyl-CoA decarboxylase, mitochondrial

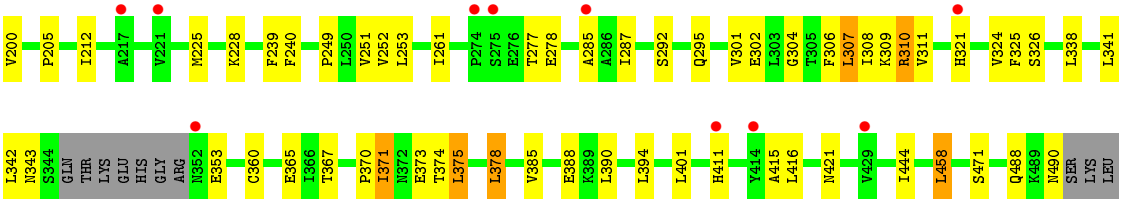
Chain B:



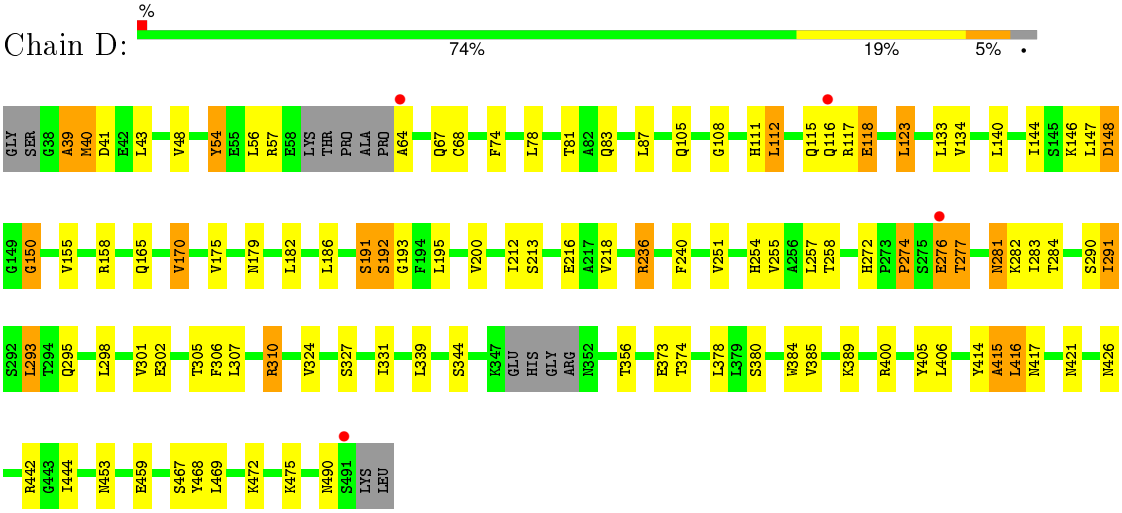
- Molecule 1: Malonyl-CoA decarboxylase, mitochondrial

Chain C:

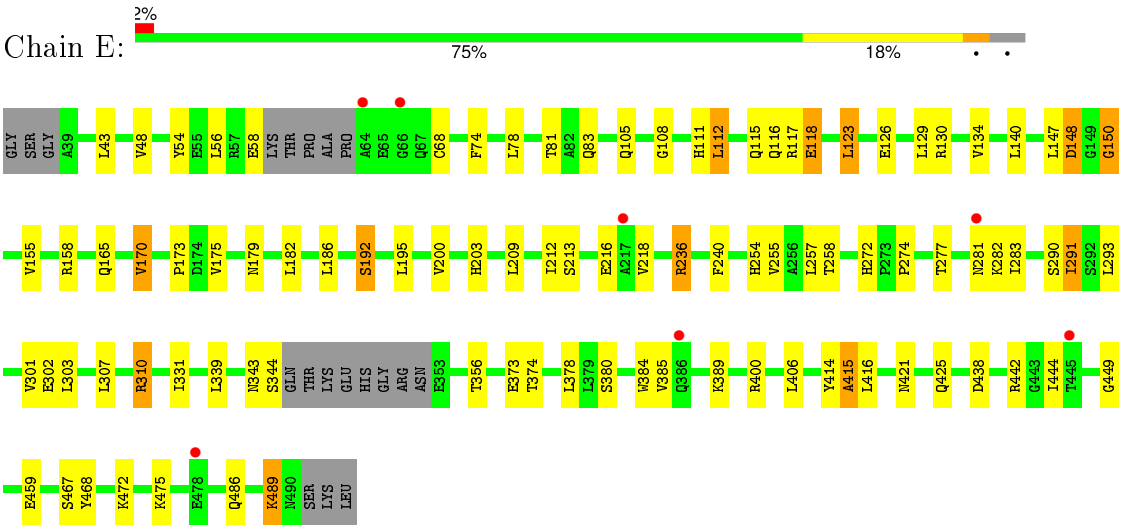




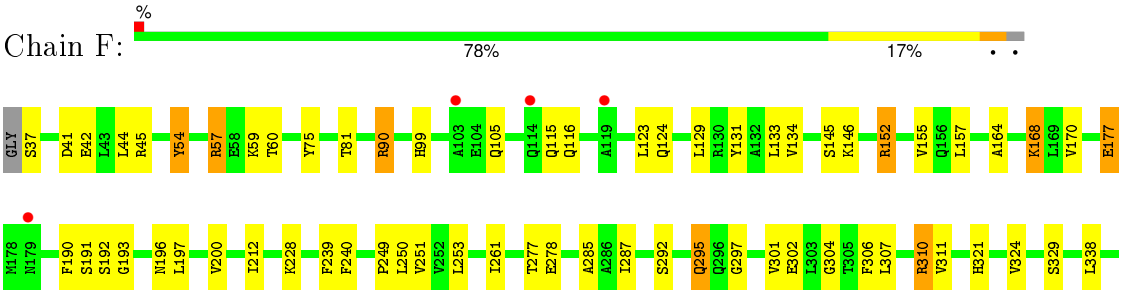
• Molecule 1: Malonyl-CoA decarboxylase, mitochondrial

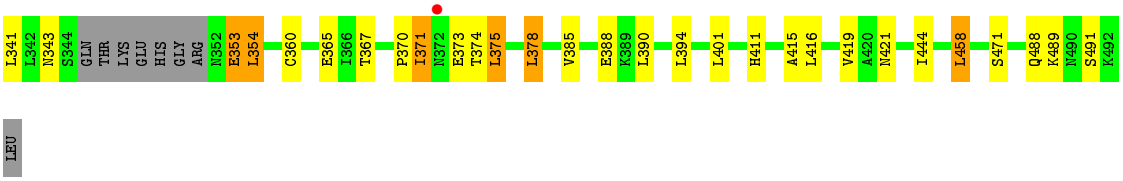


• Molecule 1: Malonyl-CoA decarboxylase, mitochondrial



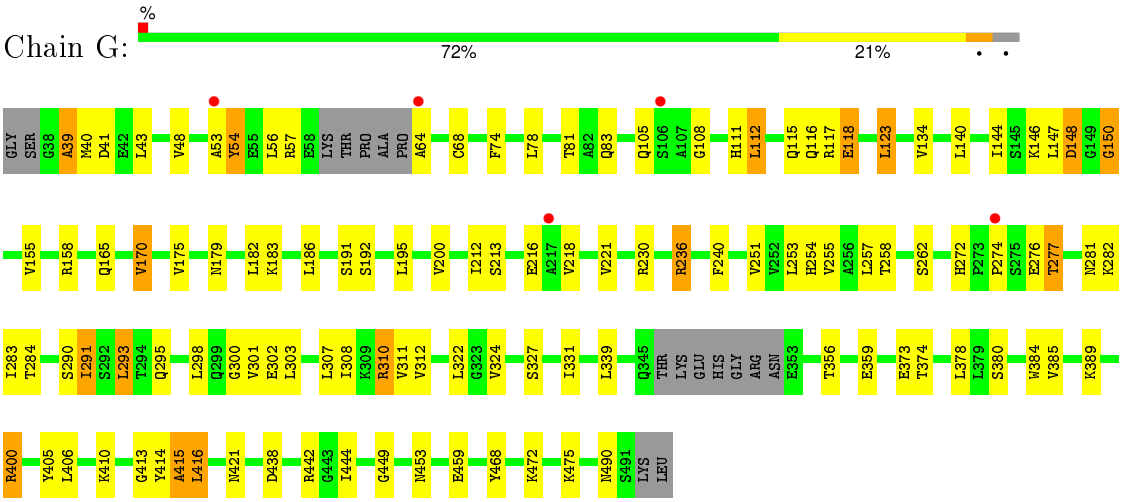
• Molecule 1: Malonyl-CoA decarboxylase, mitochondrial





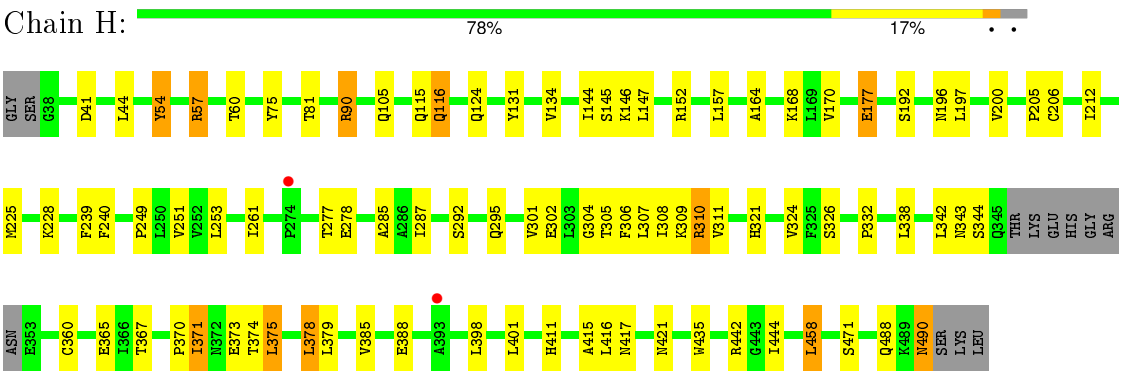
- Molecule 1: Malonyl-CoA decarboxylase, mitochondrial

Chain G:



- Molecule 1: Malonyl-CoA decarboxylase, mitochondrial

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	80.42Å 103.31Å 134.24Å 95.32° 90.22° 94.46°	Depositor
Resolution (Å)	66.80 – 3.29 66.83 – 3.29	Depositor EDS
% Data completeness (in resolution range)	98.2 (66.80-3.29) 76.5 (66.83-3.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 3.26Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.244 , 0.267 0.257 , 0.273	Depositor DCC
R_{free} test set	3242 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	51.9	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 2.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 63973 reflections	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	28107	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.05% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 0OR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.44	0/3661	0.74	0/4958
1	B	0.44	0/3540	0.74	0/4790
1	C	0.43	0/3581	0.72	0/4849
1	D	0.45	0/3570	0.74	0/4831
1	E	0.44	0/3536	0.73	1/4785 (0.0%)
1	F	0.44	0/3603	0.73	1/4879 (0.0%)
1	G	0.44	0/3550	0.74	1/4804 (0.0%)
1	H	0.44	0/3588	0.73	0/4858
All	All	0.44	0/28629	0.73	3/38754 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	64	ALA	N-CA-C	6.28	127.95	111.00
1	E	58	GLU	N-CA-C	5.67	126.30	111.00
1	F	37	SER	C-N-CA	5.10	133.01	122.30

There are no chirality outliers.

There are no planarity outliers.

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	3581	0	3587	46	0
1	B	3465	0	3473	47	0
1	C	3503	0	3509	48	0
1	D	3495	0	3490	64	0
1	E	3461	0	3470	49	0
1	F	3525	0	3528	48	0
1	G	3475	0	3477	62	0
1	H	3510	0	3524	46	0
2	B	23	0	20	2	0
2	D	23	0	20	2	0
2	E	23	0	20	2	0
2	G	23	0	20	4	0
All	All	28107	0	28138	381	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (381) 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:F:131:TYR:O	1:F:134:VAL:HG12	1.81	0.80
1:C:177:GLU:HG3	1:D:123:LEU:HD21	1.65	0.79
1:H:200:VAL:HG21	1:H:212:ILE:CD1	2.14	0.78
1:G:123:LEU:HD21	1:H:177:GLU:HG3	1.67	0.77
1:F:200:VAL:HG21	1:F:212:ILE:CD1	2.15	0.76
1:C:200:VAL:HG21	1:C:212:ILE:CD1	2.15	0.76
1:A:200:VAL:HG21	1:A:212:ILE:CD1	2.17	0.74
1:H:306:PHE:O	1:H:310:ARG:HB2	1.87	0.74
1:A:131:TYR:O	1:A:134:VAL:HG12	1.88	0.73
1:C:131:TYR:O	1:C:134:VAL:HG12	1.88	0.73
1:H:131:TYR:O	1:H:134:VAL:HG12	1.89	0.72
1:F:304:GLY:HA2	1:F:307:LEU:HD12	1.72	0.72
1:E:158:ARG:NH1	1:E:179:ASN:OD1	2.23	0.72
1:H:253:LEU:HD23	1:H:311:VAL:HG21	1.72	0.71
1:G:251:VAL:HG13	1:G:307:LEU:HD22	1.72	0.71
1:G:158:ARG:NH1	1:G:179:ASN:OD1	2.24	0.70
1:D:276:GLU:O	1:D:277:THR:O	2.09	0.70
1:D:421:ASN:ND2	1:D:468:TYR:OH	2.23	0.70
1:E:374:THR:O	1:E:378:LEU:HD23	1.92	0.70
1:B:158:ARG:NH1	1:B:179:ASN:OD1	2.25	0.69
1:H:338:LEU:HD11	1:H:401:LEU:HD13	1.74	0.69
1:H:304:GLY:HA2	1:H:307:LEU:HD12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:VAL:HG13	1:D:307:LEU:HD22	1.74	0.68
1:A:200:VAL:HG21	1:A:212:ILE:HD12	1.75	0.68
1:D:158:ARG:NH1	1:D:179:ASN:OD1	2.27	0.68
1:F:45:ARG:HG3	1:F:45:ARG:HH11	1.60	0.67
1:E:165:GLN:HE21	1:E:175:VAL:HG23	1.58	0.67
1:B:374:THR:O	1:B:378:LEU:HD23	1.96	0.66
1:C:200:VAL:HG21	1:C:212:ILE:HD12	1.77	0.66
1:F:200:VAL:HG21	1:F:212:ILE:HD12	1.76	0.66
1:D:374:THR:O	1:D:378:LEU:HD23	1.95	0.66
1:C:177:GLU:HG3	1:D:123:LEU:CD2	2.26	0.66
1:G:421:ASN:ND2	1:G:468:TYR:OH	2.28	0.65
1:B:421:ASN:ND2	1:B:468:TYR:OH	2.30	0.65
1:G:302:GLU:OE2	1:H:60:THR:HG23	1.96	0.65
1:B:165:GLN:HE21	1:B:175:VAL:HG23	1.61	0.65
1:A:177:GLU:OE2	1:B:123:LEU:HD21	1.97	0.64
1:D:68:CYS:HB2	1:D:147:LEU:HD21	1.78	0.64
1:C:253:LEU:HD23	1:C:311:VAL:HG21	1.80	0.64
1:E:123:LEU:HD21	1:F:177:GLU:OE2	1.98	0.64
1:D:378:LEU:HD12	1:D:384:TRP:HB3	1.80	0.63
1:H:200:VAL:HG21	1:H:212:ILE:HD12	1.81	0.63
1:B:200:VAL:HG21	1:B:212:ILE:HD12	1.79	0.63
1:B:378:LEU:HD12	1:B:384:TRP:HB3	1.81	0.63
1:D:165:GLN:HE21	1:D:175:VAL:HG23	1.62	0.63
1:E:68:CYS:HB2	1:E:147:LEU:HD21	1.81	0.62
1:G:200:VAL:HG21	1:G:212:ILE:HD12	1.81	0.62
1:C:338:LEU:HD11	1:C:401:LEU:HD13	1.82	0.62
1:B:251:VAL:HG13	1:B:307:LEU:HD22	1.80	0.62
1:A:285:ALA:HB2	1:A:324:VAL:HB	1.82	0.61
1:E:200:VAL:HG21	1:E:212:ILE:HD12	1.80	0.61
1:B:68:CYS:HB2	1:B:147:LEU:HD21	1.81	0.61
1:D:78:LEU:HD22	1:D:83:GLN:HB3	1.81	0.61
1:A:306:PHE:O	1:A:310:ARG:HB2	2.01	0.61
1:D:200:VAL:HG21	1:D:212:ILE:HD12	1.81	0.61
1:E:421:ASN:ND2	1:E:468:TYR:OH	2.34	0.61
1:G:165:GLN:HE21	1:G:175:VAL:HG23	1.64	0.61
1:F:458:LEU:H	1:F:458:LEU:HD12	1.66	0.61
1:H:385:VAL:HG11	1:H:444:ILE:HD12	1.83	0.60
1:D:385:VAL:HG11	1:D:444:ILE:HD12	1.83	0.60
1:C:304:GLY:HA2	1:C:307:LEU:HD22	1.84	0.59
1:G:374:THR:O	1:G:378:LEU:HD23	2.00	0.59
1:E:425:GLN:NE2	1:F:59:LYS:HD3	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LEU:HD23	1:A:311:VAL:HG21	1.83	0.59
1:A:123:LEU:HD12	1:B:173:PRO:HB2	1.84	0.59
1:D:236:ARG:HB2	1:D:255:VAL:HB	1.84	0.59
1:G:78:LEU:HD22	1:G:83:GLN:HB3	1.85	0.59
1:E:378:LEU:HD12	1:E:384:TRP:HB3	1.86	0.58
1:D:117:ARG:O	1:D:118:GLU:O	2.22	0.58
1:A:152:ARG:NH2	1:A:295:GLN:OE1	2.36	0.58
1:G:39:ALA:O	1:G:41:ASP:N	2.37	0.58
1:E:486:GLN:HA	1:E:489:LYS:HD3	1.84	0.58
1:G:378:LEU:HD12	1:G:384:TRP:HB3	1.86	0.58
1:A:304:GLY:HA2	1:A:307:LEU:HD23	1.85	0.58
1:A:486:GLN:HA	1:A:489:LYS:HE2	1.86	0.57
1:B:78:LEU:HD22	1:B:83:GLN:HB3	1.86	0.57
1:E:78:LEU:HD22	1:E:83:GLN:HB3	1.85	0.57
1:G:331:ILE:HG23	1:G:406:LEU:HD21	1.86	0.56
1:B:236:ARG:HB2	1:B:255:VAL:HB	1.87	0.56
1:A:59:LYS:HD3	1:B:425:GLN:HE21	1.70	0.56
1:E:425:GLN:HE21	1:F:59:LYS:HD3	1.70	0.56
1:C:285:ALA:HB2	1:C:324:VAL:HB	1.87	0.56
1:G:385:VAL:HG11	1:G:444:ILE:HD12	1.87	0.56
1:B:192:SER:HA	1:B:195:LEU:HD12	1.88	0.56
1:H:200:VAL:HG21	1:H:212:ILE:HD11	1.85	0.56
1:G:123:LEU:CD2	1:H:177:GLU:HG3	2.34	0.56
1:A:60:THR:HG23	1:B:302:GLU:OE2	2.05	0.56
1:G:68:CYS:HB2	1:G:147:LEU:HD21	1.88	0.55
1:B:291:ILE:HG23	2:B:501[A]:0OR:C39	2.36	0.55
1:C:385:VAL:HG11	1:C:444:ILE:HD12	1.87	0.55
1:E:236:ARG:HB2	1:E:255:VAL:HB	1.87	0.55
1:D:305:THR:HG23	1:D:426:ASN:ND2	2.21	0.55
1:E:343:ASN:HA	1:E:344:SER:CB	2.36	0.55
1:E:170:VAL:HB	1:E:175:VAL:HG11	1.89	0.55
1:B:170:VAL:HB	1:B:175:VAL:HG11	1.89	0.55
1:D:331:ILE:HG23	1:D:406:LEU:HD21	1.89	0.55
1:H:60:THR:HG21	1:H:146:LYS:NZ	2.22	0.54
1:E:173:PRO:HB2	1:F:123:LEU:HD12	1.88	0.54
1:D:192:SER:HA	1:D:195:LEU:HD12	1.88	0.54
1:A:485:ALA:O	1:A:489:LYS:HG3	2.07	0.54
1:A:60:THR:HG21	1:A:146:LYS:NZ	2.23	0.54
1:C:458:LEU:H	1:C:458:LEU:HD12	1.73	0.54
1:C:200:VAL:HG21	1:C:212:ILE:HD11	1.88	0.54
1:A:458:LEU:HD12	1:A:458:LEU:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:VAL:HG11	1:C:444:ILE:CD1	2.38	0.54
1:D:293:LEU:HD12	2:D:501[A]:0OR:H5	1.89	0.54
1:G:302:GLU:HA	2:G:501[A]:0OR:O21	2.08	0.54
1:H:332:PRO:O	1:H:417:ASN:ND2	2.40	0.54
1:F:253:LEU:HD23	1:F:311:VAL:HG21	1.90	0.54
1:F:190:PHE:HE1	1:F:250:LEU:HD21	1.73	0.54
1:B:385:VAL:HG11	1:B:444:ILE:HD12	1.90	0.53
1:A:59:LYS:HD3	1:B:425:GLN:NE2	2.23	0.53
1:E:302:GLU:OE2	1:F:60:THR:HG23	2.08	0.53
1:H:458:LEU:H	1:H:458:LEU:HD12	1.72	0.53
1:H:490:ASN:H	1:H:490:ASN:HD22	1.54	0.53
1:D:414:TYR:O	1:D:415:ALA:CB	2.57	0.53
1:G:236:ARG:HB2	1:G:255:VAL:HB	1.90	0.53
1:G:170:VAL:HB	1:G:175:VAL:HG11	1.89	0.53
1:D:170:VAL:HB	1:D:175:VAL:HG11	1.89	0.53
1:A:191:SER:O	1:A:193:GLY:N	2.42	0.52
1:F:354:LEU:CD2	1:F:401:LEU:HD21	2.39	0.52
1:A:190:PHE:HE1	1:A:250:LEU:HD21	1.73	0.52
1:D:191:SER:O	1:D:193:GLY:N	2.43	0.52
1:D:339:LEU:HD11	1:D:380:SER:HB3	1.92	0.52
1:A:240:PHE:CD1	1:A:307:LEU:HD12	2.44	0.52
1:H:385:VAL:HG11	1:H:444:ILE:CD1	2.40	0.52
1:C:130:ARG:NH1	1:D:133:LEU:O	2.43	0.52
1:E:302:GLU:HA	2:E:501[A]:0OR:O21	2.10	0.51
1:E:385:VAL:HG11	1:E:444:ILE:HD12	1.93	0.51
1:A:338:LEU:HD11	1:A:401:LEU:HD13	1.93	0.51
1:E:331:ILE:HG23	1:E:406:LEU:HD21	1.92	0.51
1:A:360:CYS:HA	1:A:371:ILE:HD13	1.93	0.51
1:E:155:VAL:HG22	1:E:186:LEU:CD2	2.40	0.51
1:C:60:THR:HG21	1:C:146:LYS:NZ	2.26	0.51
1:D:155:VAL:HG11	1:D:295:GLN:HG2	1.93	0.51
1:F:385:VAL:HG11	1:F:444:ILE:HD12	1.93	0.51
1:E:414:TYR:O	1:E:415:ALA:HB3	2.11	0.50
1:H:164:ALA:HB1	1:H:170:VAL:HG22	1.93	0.50
1:H:285:ALA:HB2	1:H:324:VAL:HB	1.93	0.50
1:G:359:GLU:OE1	1:G:400:ARG:NH2	2.45	0.50
1:E:117:ARG:O	1:E:118:GLU:O	2.29	0.50
1:G:117:ARG:O	1:G:118:GLU:O	2.30	0.50
1:B:117:ARG:O	1:B:118:GLU:O	2.29	0.50
1:H:411:HIS:HB2	1:H:416:LEU:HD12	1.94	0.50
1:D:414:TYR:O	1:D:415:ALA:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:HIS:HB2	1:C:416:LEU:HD12	1.93	0.50
1:F:60:THR:HG21	1:F:146:LYS:NZ	2.27	0.50
1:C:164:ALA:HB1	1:C:170:VAL:HG22	1.94	0.50
1:F:200:VAL:HG21	1:F:212:ILE:HD11	1.90	0.50
1:D:459:GLU:CD	1:D:459:GLU:H	2.15	0.50
1:F:45:ARG:HG3	1:F:45:ARG:NH1	2.26	0.49
1:E:414:TYR:O	1:E:468:TYR:OH	2.23	0.49
1:B:414:TYR:O	1:B:415:ALA:CB	2.60	0.49
1:G:195:LEU:O	1:G:310:ARG:NH2	2.45	0.49
1:E:459:GLU:CD	1:E:459:GLU:H	2.15	0.49
1:D:274:PRO:CB	1:D:276:GLU:HG2	2.42	0.49
1:E:192:SER:HA	1:E:195:LEU:HD12	1.95	0.49
1:G:414:TYR:O	1:G:415:ALA:HB3	2.13	0.49
1:A:164:ALA:HB1	1:A:170:VAL:HG22	1.94	0.49
1:F:329:SER:HB3	1:F:419:VAL:HG11	1.92	0.49
1:A:411:HIS:HB2	1:A:416:LEU:HD12	1.93	0.49
1:E:291:ILE:HG23	2:E:501[A]:0OR:C39	2.42	0.49
1:B:39:ALA:O	1:B:41:ASP:N	2.46	0.49
1:F:360:CYS:HA	1:F:371:ILE:HD13	1.95	0.49
1:A:385:VAL:HG11	1:A:444:ILE:HD12	1.95	0.49
1:H:305:THR:HG23	1:H:309:LYS:HE3	1.95	0.49
1:D:274:PRO:HB2	1:D:276:GLU:CG	2.43	0.49
1:B:257:LEU:HD13	1:B:283:ILE:HD13	1.95	0.49
1:D:257:LEU:HD13	1:D:283:ILE:HD13	1.94	0.49
1:H:251:VAL:HA	1:H:292:SER:O	2.13	0.49
1:B:414:TYR:O	1:B:415:ALA:HB3	2.13	0.49
1:B:302:GLU:HA	2:B:501[A]:0OR:O21	2.13	0.48
1:G:414:TYR:O	1:G:415:ALA:CB	2.61	0.48
1:F:338:LEU:HD11	1:F:401:LEU:HD13	1.95	0.48
1:D:301:VAL:HG12	1:D:301:VAL:O	2.13	0.48
1:F:164:ALA:HB1	1:F:170:VAL:HG22	1.95	0.48
1:E:414:TYR:O	1:E:415:ALA:CB	2.61	0.48
1:C:177:GLU:OE2	1:D:123:LEU:HD21	2.13	0.48
1:F:285:ALA:HB2	1:F:324:VAL:HB	1.96	0.48
1:B:459:GLU:CD	1:B:459:GLU:H	2.16	0.48
1:G:192:SER:HA	1:G:195:LEU:HD12	1.95	0.48
1:F:411:HIS:HB2	1:F:416:LEU:HD12	1.94	0.48
1:G:155:VAL:HG11	1:G:295:GLN:HG2	1.94	0.48
1:A:371:ILE:HG13	1:A:375:LEU:CD2	2.43	0.48
1:E:155:VAL:HG22	1:E:186:LEU:HD21	1.95	0.48
1:B:339:LEU:CD2	1:B:376:LYS:HA	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:CYS:HA	1:C:371:ILE:HD13	1.94	0.48
1:H:360:CYS:HA	1:H:371:ILE:HD13	1.94	0.48
1:B:155:VAL:HG22	1:B:186:LEU:CD2	2.44	0.47
1:A:200:VAL:HG21	1:A:212:ILE:HD11	1.92	0.47
1:G:155:VAL:HG22	1:G:186:LEU:CD2	2.44	0.47
1:B:414:TYR:CE1	1:B:472:LYS:HG2	2.49	0.47
1:D:155:VAL:HG22	1:D:186:LEU:CD2	2.45	0.47
1:G:54:TYR:O	1:G:57:ARG:HB3	2.14	0.47
1:G:301:VAL:HG12	1:G:301:VAL:O	2.14	0.47
1:G:327:SER:O	1:G:453:ASN:ND2	2.40	0.47
1:E:129:LEU:HD21	1:F:129:LEU:HD21	1.97	0.47
1:G:213:SER:O	1:G:216:GLU:HB3	2.14	0.47
1:F:191:SER:O	1:F:193:GLY:N	2.48	0.47
1:A:287:ILE:HA	1:A:326:SER:O	2.15	0.47
1:E:200:VAL:HG21	1:E:212:ILE:CD1	2.43	0.47
1:H:490:ASN:HD22	1:H:490:ASN:N	2.13	0.47
1:E:257:LEU:HD13	1:E:283:ILE:HD13	1.97	0.47
1:B:301:VAL:HG12	1:B:301:VAL:O	2.14	0.47
1:G:200:VAL:HG21	1:G:212:ILE:CD1	2.45	0.47
1:F:152:ARG:NH2	1:F:295:GLN:OE1	2.45	0.47
1:D:414:TYR:CE1	1:D:472:LYS:HG2	2.49	0.47
1:D:186:LEU:HD22	1:D:298:LEU:CD2	2.45	0.47
1:H:371:ILE:HG13	1:H:375:LEU:CD2	2.45	0.46
1:B:148:ASP:C	1:B:150:GLY:H	2.19	0.46
1:H:305:THR:CG2	1:H:309:LYS:HE3	2.45	0.46
1:D:254:HIS:HB2	1:D:290:SER:HB3	1.97	0.46
1:C:177:GLU:CG	1:D:123:LEU:HD21	2.40	0.46
1:C:307:LEU:O	1:C:311:VAL:HG23	2.15	0.46
1:H:261:ILE:HA	1:H:287:ILE:HD11	1.96	0.46
1:G:148:ASP:C	1:G:150:GLY:H	2.18	0.46
1:D:54:TYR:O	1:D:57:ARG:HB3	2.16	0.46
1:D:144:ILE:HA	1:D:147:LEU:HD22	1.96	0.46
1:B:155:VAL:HG22	1:B:186:LEU:HD21	1.98	0.46
1:G:43:LEU:HD22	1:G:74:PHE:CG	2.50	0.46
1:B:200:VAL:HG21	1:B:212:ILE:CD1	2.45	0.46
1:D:324:VAL:HG21	1:G:284:THR:HG21	1.98	0.46
1:G:257:LEU:HD13	1:G:283:ILE:HD13	1.97	0.46
1:C:60:THR:HG23	1:D:302:GLU:OE2	2.15	0.46
1:D:39:ALA:O	1:D:41:ASP:N	2.48	0.46
1:A:338:LEU:HD23	1:A:379:LEU:HD13	1.98	0.46
1:E:301:VAL:O	1:E:301:VAL:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:LEU:HD22	1:E:74:PHE:CG	2.51	0.45
1:A:251:VAL:HA	1:A:292:SER:O	2.16	0.45
1:F:371:ILE:HG13	1:F:375:LEU:CD2	2.46	0.45
1:D:43:LEU:HD22	1:D:74:PHE:CG	2.51	0.45
1:G:308:ILE:O	1:G:312:VAL:HG23	2.15	0.45
1:G:339:LEU:HD11	1:G:380:SER:HB3	1.99	0.45
1:B:43:LEU:HD22	1:B:74:PHE:CG	2.51	0.45
1:D:200:VAL:HG21	1:D:212:ILE:CD1	2.47	0.45
1:B:54:TYR:O	1:B:57:ARG:HB3	2.16	0.45
1:B:203:HIS:O	1:C:205:PRO:HB3	2.16	0.45
1:D:155:VAL:HG22	1:D:186:LEU:HD21	1.99	0.45
1:C:371:ILE:HG13	1:C:375:LEU:CD2	2.46	0.45
1:F:251:VAL:HA	1:F:292:SER:O	2.17	0.45
1:C:341:LEU:C	1:C:343:ASN:H	2.19	0.45
1:D:274:PRO:HB3	1:D:276:GLU:HG2	1.98	0.45
1:G:400:ARG:NH1	1:G:490:ASN:OD1	2.50	0.45
1:G:108:GLY:O	1:G:112:LEU:HD12	2.16	0.45
1:E:148:ASP:C	1:E:150:GLY:H	2.18	0.45
1:A:196:ASN:O	1:A:240:PHE:HA	2.17	0.44
1:H:44:LEU:CD1	1:H:90:ARG:HB3	2.47	0.44
1:E:213:SER:O	1:E:216:GLU:HB3	2.17	0.44
1:A:352:ASN:CG	1:A:372:ASN:HD21	2.20	0.44
1:G:459:GLU:H	1:G:459:GLU:CD	2.20	0.44
1:F:341:LEU:O	1:F:343:ASN:N	2.50	0.44
1:D:195:LEU:O	1:D:310:ARG:NH2	2.50	0.44
1:E:339:LEU:HD11	1:E:380:SER:HB3	2.00	0.44
1:E:203:HIS:O	1:H:205:PRO:HB3	2.16	0.44
1:A:374:THR:HG22	1:A:378:LEU:HD11	1.98	0.44
1:D:148:ASP:C	1:D:150:GLY:H	2.20	0.44
1:A:261:ILE:HA	1:A:287:ILE:HD11	1.98	0.44
1:G:414:TYR:CE1	1:G:472:LYS:HG2	2.53	0.44
1:E:414:TYR:CE1	1:E:472:LYS:HG2	2.53	0.44
1:C:367:THR:OG1	1:C:374:THR:HG21	2.18	0.44
1:B:331:ILE:HG23	1:B:406:LEU:HD21	1.98	0.44
1:C:44:LEU:CD1	1:C:90:ARG:HB3	2.48	0.44
1:E:254:HIS:HB2	1:E:290:SER:HB3	1.99	0.44
1:G:186:LEU:HD22	1:G:298:LEU:CD2	2.48	0.44
1:H:374:THR:HG22	1:H:378:LEU:HD11	2.00	0.44
1:G:254:HIS:HB2	1:G:290:SER:HB3	2.00	0.44
1:G:414:TYR:HB3	1:G:421:ASN:ND2	2.33	0.44
1:C:338:LEU:CD1	1:C:401:LEU:HD13	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:458:LEU:N	1:F:458:LEU:HD12	2.32	0.44
1:A:197:LEU:HD13	1:A:240:PHE:CZ	2.52	0.44
1:C:287:ILE:HA	1:C:326:SER:O	2.18	0.44
1:D:405:TYR:CE1	1:D:416:LEU:HD23	2.53	0.44
1:H:144:ILE:O	1:H:147:LEU:HB2	2.18	0.44
1:A:367:THR:OG1	1:A:374:THR:HG21	2.18	0.43
1:F:374:THR:HG22	1:F:378:LEU:HD11	1.99	0.43
1:D:48:VAL:HA	1:D:140:LEU:HD13	2.00	0.43
1:B:108:GLY:O	1:B:112:LEU:HD12	2.18	0.43
1:B:414:TYR:HB3	1:B:421:ASN:ND2	2.33	0.43
1:F:354:LEU:HD22	1:F:401:LEU:HD21	1.99	0.43
1:H:305:THR:HG23	1:H:309:LYS:CE	2.48	0.43
1:F:196:ASN:O	1:F:240:PHE:HA	2.18	0.43
1:F:306:PHE:O	1:F:310:ARG:HB2	2.18	0.43
1:C:251:VAL:HA	1:C:292:SER:O	2.19	0.43
1:H:54:TYR:O	1:H:57:ARG:HB3	2.19	0.43
1:G:405:TYR:CE1	1:G:416:LEU:HD23	2.53	0.43
1:B:213:SER:O	1:B:216:GLU:HB3	2.18	0.43
1:C:212:ILE:HG23	1:C:252:VAL:HG11	2.00	0.43
1:B:236:ARG:HD3	1:B:236:ARG:HA	1.85	0.43
1:C:261:ILE:HA	1:C:287:ILE:HD11	1.99	0.43
1:H:75:TYR:CZ	1:H:157:LEU:HD12	2.53	0.43
1:H:338:LEU:HD23	1:H:379:LEU:HD13	2.01	0.43
1:A:346:THR:HG23	1:A:372:ASN:HB3	2.01	0.43
1:C:55:GLU:N	1:C:55:GLU:OE1	2.52	0.43
1:G:438:ASP:O	1:G:449:GLY:HA2	2.18	0.43
1:H:338:LEU:CD1	1:H:401:LEU:HD13	2.45	0.43
1:E:48:VAL:HA	1:E:140:LEU:HD13	2.00	0.43
1:G:291:ILE:HG23	2:G:501[A]:0OR:C39	2.48	0.43
1:H:196:ASN:O	1:H:240:PHE:HA	2.19	0.43
1:F:44:LEU:CD1	1:F:90:ARG:HB3	2.48	0.43
1:E:130:ARG:HH11	1:F:133:LEU:HB3	1.84	0.43
1:B:359:GLU:OE1	1:B:400:ARG:NH2	2.50	0.43
1:H:307:LEU:O	1:H:311:VAL:HG23	2.19	0.43
1:E:68:CYS:HB2	1:E:147:LEU:CD2	2.48	0.43
1:F:367:THR:OG1	1:F:374:THR:HG21	2.19	0.43
1:D:64:ALA:HA	1:D:67:GLN:HB2	2.01	0.43
1:C:183:LYS:HG3	1:C:301:VAL:HG22	2.01	0.42
1:B:415:ALA:O	1:B:417:ASN:N	2.52	0.42
1:B:144:ILE:O	1:B:147:LEU:HB2	2.20	0.42
1:F:354:LEU:HD22	1:F:401:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:THR:HG22	1:C:378:LEU:HD11	2.00	0.42
1:G:221:VAL:HG22	1:G:230:ARG:CZ	2.49	0.42
1:D:213:SER:O	1:D:216:GLU:HB3	2.20	0.42
1:D:281:ASN:OD1	1:D:281:ASN:N	2.50	0.42
1:D:108:GLY:O	1:D:112:LEU:HD12	2.19	0.42
1:F:385:VAL:HG11	1:F:444:ILE:CD1	2.50	0.42
1:G:155:VAL:HG22	1:G:186:LEU:HD21	2.01	0.42
1:B:254:HIS:HB2	1:B:290:SER:HB3	2.00	0.42
1:D:40:MET:HG3	1:D:87:LEU:HD13	2.01	0.42
1:G:253:LEU:HD23	1:G:311:VAL:HG21	2.01	0.42
1:C:239:PHE:CD1	1:C:249:PRO:HB3	2.54	0.42
1:G:48:VAL:HA	1:G:140:LEU:HD13	2.01	0.42
1:C:304:GLY:O	1:C:307:LEU:HB2	2.20	0.42
1:E:195:LEU:O	1:E:310:ARG:NH2	2.52	0.42
1:F:197:LEU:HD13	1:F:240:PHE:CZ	2.54	0.42
1:A:390:LEU:HG	1:A:394:LEU:HD12	2.02	0.42
1:A:44:LEU:CD1	1:A:90:ARG:HB3	2.49	0.42
1:C:56:LEU:HD22	1:D:469:LEU:HB3	2.01	0.42
1:H:367:THR:OG1	1:H:374:THR:HG21	2.20	0.42
1:C:325:PHE:HE2	1:C:458:LEU:HD21	1.85	0.42
1:A:458:LEU:N	1:A:458:LEU:HD12	2.34	0.42
1:F:155:VAL:HG13	1:F:297:GLY:HA3	2.01	0.42
1:F:239:PHE:CD1	1:F:249:PRO:HB3	2.55	0.42
1:B:221:VAL:HG22	1:B:230:ARG:CZ	2.49	0.42
1:H:251:VAL:HG22	1:H:253:LEU:CD1	2.50	0.42
1:D:291:ILE:HG23	2:D:501[A]:0OR:C39	2.50	0.42
1:C:146:LYS:HZ3	1:D:306:PHE:HZ	1.66	0.42
1:C:306:PHE:O	1:C:310:ARG:HB2	2.20	0.42
1:C:75:TYR:CZ	1:C:157:LEU:HD12	2.55	0.42
1:H:458:LEU:N	1:H:458:LEU:HD12	2.34	0.41
1:C:458:LEU:N	1:C:458:LEU:HD12	2.34	0.41
1:D:415:ALA:O	1:D:417:ASN:N	2.53	0.41
1:A:338:LEU:CD1	1:A:401:LEU:HD13	2.50	0.41
1:H:287:ILE:HA	1:H:326:SER:O	2.20	0.41
1:D:144:ILE:O	1:D:147:LEU:HB2	2.20	0.41
1:G:236:ARG:HD3	1:G:236:ARG:HA	1.84	0.41
1:C:196:ASN:O	1:C:240:PHE:HA	2.20	0.41
1:D:327:SER:O	1:D:453:ASN:ND2	2.42	0.41
1:A:54:TYR:O	1:A:57:ARG:HB3	2.20	0.41
1:G:283:ILE:HG22	1:G:322:LEU:HD13	2.02	0.41
1:C:44:LEU:HD11	1:C:90:ARG:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:LEU:HD23	1:H:206:CYS:SG	2.60	0.41
1:F:75:TYR:CZ	1:F:157:LEU:HD12	2.56	0.41
1:G:155:VAL:CG1	1:G:295:GLN:HG2	2.50	0.41
1:G:144:ILE:O	1:G:147:LEU:HB2	2.20	0.41
1:E:236:ARG:HD3	1:E:236:ARG:HA	1.86	0.41
1:G:405:TYR:HE1	1:G:416:LEU:HD23	1.85	0.41
1:G:183:LYS:HE3	1:G:300:GLY:O	2.21	0.41
1:F:390:LEU:HG	1:F:394:LEU:HD12	2.03	0.41
1:G:291:ILE:HG13	2:G:501[A]:0OR:H9	2.03	0.41
1:C:197:LEU:HD13	1:C:240:PHE:CZ	2.56	0.41
1:E:438:ASP:O	1:E:449:GLY:HA2	2.20	0.41
1:A:239:PHE:CD1	1:A:249:PRO:HB3	2.56	0.41
1:F:261:ILE:HA	1:F:287:ILE:HD11	2.01	0.41
1:C:390:LEU:HG	1:C:394:LEU:HD12	2.02	0.41
1:A:75:TYR:CZ	1:A:157:LEU:HD12	2.56	0.41
1:D:186:LEU:HD22	1:D:298:LEU:HD23	2.04	0.40
1:H:197:LEU:HD13	1:H:240:PHE:CZ	2.56	0.40
1:F:54:TYR:O	1:F:57:ARG:HB3	2.21	0.40
1:E:126:GLU:CD	1:F:99:HIS:HD1	2.22	0.40
1:E:108:GLY:O	1:E:112:LEU:HD12	2.21	0.40
1:G:410:LYS:HB3	1:G:413:GLY:HA2	2.03	0.40
1:D:284:THR:HG21	1:G:324:VAL:CG2	2.51	0.40
1:G:293:LEU:HD12	2:G:501[A]:0OR:H5	2.04	0.40
1:D:68:CYS:HB2	1:D:147:LEU:CD2	2.49	0.40
1:H:398:LEU:HD12	1:H:435:TRP:HH2	1.86	0.40
1:B:68:CYS:HB2	1:B:147:LEU:CD2	2.51	0.40
1:G:276:GLU:O	1:G:277:THR:O	2.39	0.40
1:A:144:ILE:HA	1:A:147:LEU:HD13	2.02	0.40
1:A:285:ALA:CB	1:A:324:VAL:HB	2.50	0.40
1:C:144:ILE:HA	1:C:147:LEU:HD13	2.03	0.40
1:H:239:PHE:CD1	1:H:249:PRO:HB3	2.57	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	454/458 (99%)	402 (88%)	42 (9%)	10 (2%)	8 41
1	B	434/458 (95%)	389 (90%)	31 (7%)	14 (3%)	5 31
1	C	442/458 (96%)	400 (90%)	30 (7%)	12 (3%)	6 35
1	D	439/458 (96%)	393 (90%)	32 (7%)	14 (3%)	5 31
1	E	433/458 (94%)	390 (90%)	32 (7%)	11 (2%)	7 37
1	F	445/458 (97%)	396 (89%)	39 (9%)	10 (2%)	8 41
1	G	436/458 (95%)	390 (89%)	33 (8%)	13 (3%)	5 33
1	H	442/458 (96%)	397 (90%)	37 (8%)	8 (2%)	11 46
All	All	3525/3664 (96%)	3157 (90%)	276 (8%)	92 (3%)	7 36

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	SER
1	A	349	HIS
1	A	371	ILE
1	B	39	ALA
1	B	40	MET
1	B	118	GLU
1	B	218	VAL
1	B	277	THR
1	B	415	ALA
1	B	416	LEU
1	C	192	SER
1	C	342	LEU
1	C	353	GLU
1	C	370	PRO
1	C	371	ILE
1	D	40	MET
1	D	54	TYR
1	D	118	GLU
1	D	192	SER
1	D	218	VAL
1	D	277	THR
1	D	344	SER
1	D	415	ALA
1	D	416	LEU

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Mol	Chain	Res	Type
1	E	118	GLU
1	E	192	SER
1	E	218	VAL
1	E	277	THR
1	E	415	ALA
1	E	416	LEU
1	F	192	SER
1	F	371	ILE
1	G	39	ALA
1	G	40	MET
1	G	54	TYR
1	G	118	GLU
1	G	218	VAL
1	G	277	THR
1	G	415	ALA
1	G	416	LEU
1	H	192	SER
1	H	371	ILE
1	A	54	TYR
1	A	116	GLN
1	A	370	PRO
1	B	54	TYR
1	B	116	GLN
1	B	148	ASP
1	B	192	SER
1	C	54	TYR
1	C	116	GLN
1	D	39	ALA
1	D	116	GLN
1	D	148	ASP
1	E	54	TYR
1	E	116	GLN
1	E	148	ASP
1	F	54	TYR
1	F	116	GLN
1	F	353	GLU
1	F	370	PRO
1	G	116	GLN
1	G	148	ASP
1	H	54	TYR
1	H	116	GLN
1	H	370	PRO

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Mol	Chain	Res	Type
1	B	150	GLY
1	E	150	GLY
1	A	395	GLN
1	C	278	GLU
1	C	415	ALA
1	F	168	LYS
1	F	278	GLU
1	F	415	ALA
1	F	491	SER
1	G	53	ALA
1	H	278	GLU
1	H	415	ALA
1	A	278	GLU
1	A	415	ALA
1	B	53	ALA
1	B	274	PRO
1	C	168	LYS
1	E	274	PRO
1	G	274	PRO
1	H	343	ASN
1	A	458	LEU
1	C	308	ILE
1	C	309	LYS
1	D	274	PRO
1	G	150	GLY
1	D	150	GLY

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	382/387 (99%)	348 (91%)	34 (9%)	12 43
1	B	369/387 (95%)	342 (93%)	27 (7%)	17 53
1	C	373/387 (96%)	343 (92%)	30 (8%)	15 49
1	D	371/387 (96%)	341 (92%)	30 (8%)	15 48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	369/387 (95%)	340 (92%)	29 (8%)	15 49
1	F	375/387 (97%)	344 (92%)	31 (8%)	14 47
1	G	369/387 (95%)	340 (92%)	29 (8%)	15 49
1	H	375/387 (97%)	341 (91%)	34 (9%)	12 41
All	All	2983/3096 (96%)	2739 (92%)	244 (8%)	14 48

All (244) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASP
1	A	42	GLU
1	A	57	ARG
1	A	60	THR
1	A	81	THR
1	A	90	ARG
1	A	105	GLN
1	A	115	GLN
1	A	124	GLN
1	A	152	ARG
1	A	168	LYS
1	A	177	GLU
1	A	222	LYS
1	A	225	MET
1	A	228	LYS
1	A	277	THR
1	A	295	GLN
1	A	301	VAL
1	A	302	GLU
1	A	307	LEU
1	A	310	ARG
1	A	321	HIS
1	A	345	GLN
1	A	365	GLU
1	A	373	GLU
1	A	375	LEU
1	A	378	LEU
1	A	388	GLU
1	A	421	ASN
1	A	458	LEU
1	A	471	SER
1	A	488	GLN

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Mol	Chain	Res	Type
1	A	492	LYS
1	A	493	LEU
1	B	56	LEU
1	B	81	THR
1	B	105	GLN
1	B	111	HIS
1	B	112	LEU
1	B	115	GLN
1	B	123	LEU
1	B	134	VAL
1	B	146	LYS
1	B	170	VAL
1	B	182	LEU
1	B	236	ARG
1	B	240	PHE
1	B	258	THR
1	B	272	HIS
1	B	281	ASN
1	B	282	LYS
1	B	291	ILE
1	B	293	LEU
1	B	310	ARG
1	B	356	THR
1	B	373	GLU
1	B	389	LYS
1	B	400	ARG
1	B	442	ARG
1	B	467	SER
1	B	475	LYS
1	C	41	ASP
1	C	42	GLU
1	C	57	ARG
1	C	60	THR
1	C	81	THR
1	C	90	ARG
1	C	105	GLN
1	C	115	GLN
1	C	124	GLN
1	C	152	ARG
1	C	168	LYS
1	C	177	GLU
1	C	225	MET

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Mol	Chain	Res	Type
1	C	228	LYS
1	C	277	THR
1	C	295	GLN
1	C	302	GLU
1	C	307	LEU
1	C	310	ARG
1	C	321	HIS
1	C	365	GLU
1	C	373	GLU
1	C	375	LEU
1	C	378	LEU
1	C	388	GLU
1	C	421	ASN
1	C	458	LEU
1	C	471	SER
1	C	488	GLN
1	C	490	ASN
1	D	56	LEU
1	D	81	THR
1	D	105	GLN
1	D	111	HIS
1	D	112	LEU
1	D	115	GLN
1	D	123	LEU
1	D	134	VAL
1	D	146	LYS
1	D	170	VAL
1	D	182	LEU
1	D	191	SER
1	D	236	ARG
1	D	240	PHE
1	D	258	THR
1	D	272	HIS
1	D	276	GLU
1	D	281	ASN
1	D	282	LYS
1	D	291	ILE
1	D	293	LEU
1	D	310	ARG
1	D	356	THR
1	D	373	GLU
1	D	389	LYS

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Mol	Chain	Res	Type
1	D	400	ARG
1	D	442	ARG
1	D	467	SER
1	D	475	LYS
1	D	490	ASN
1	E	56	LEU
1	E	81	THR
1	E	105	GLN
1	E	111	HIS
1	E	112	LEU
1	E	115	GLN
1	E	123	LEU
1	E	134	VAL
1	E	170	VAL
1	E	182	LEU
1	E	236	ARG
1	E	240	PHE
1	E	258	THR
1	E	272	HIS
1	E	281	ASN
1	E	282	LYS
1	E	291	ILE
1	E	293	LEU
1	E	303	LEU
1	E	307	LEU
1	E	310	ARG
1	E	356	THR
1	E	373	GLU
1	E	389	LYS
1	E	400	ARG
1	E	442	ARG
1	E	467	SER
1	E	475	LYS
1	E	489	LYS
1	F	41	ASP
1	F	42	GLU
1	F	57	ARG
1	F	81	THR
1	F	90	ARG
1	F	105	GLN
1	F	115	GLN
1	F	124	GLN

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Mol	Chain	Res	Type
1	F	145	SER
1	F	152	ARG
1	F	168	LYS
1	F	177	GLU
1	F	228	LYS
1	F	277	THR
1	F	295	GLN
1	F	301	VAL
1	F	302	GLU
1	F	310	ARG
1	F	321	HIS
1	F	353	GLU
1	F	354	LEU
1	F	365	GLU
1	F	373	GLU
1	F	375	LEU
1	F	378	LEU
1	F	388	GLU
1	F	421	ASN
1	F	458	LEU
1	F	471	SER
1	F	488	GLN
1	F	489	LYS
1	G	56	LEU
1	G	81	THR
1	G	105	GLN
1	G	111	HIS
1	G	112	LEU
1	G	115	GLN
1	G	123	LEU
1	G	134	VAL
1	G	146	LYS
1	G	170	VAL
1	G	182	LEU
1	G	191	SER
1	G	236	ARG
1	G	240	PHE
1	G	258	THR
1	G	262	SER
1	G	272	HIS
1	G	281	ASN
1	G	282	LYS

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Mol	Chain	Res	Type
1	G	291	ILE
1	G	293	LEU
1	G	303	LEU
1	G	310	ARG
1	G	356	THR
1	G	373	GLU
1	G	389	LYS
1	G	400	ARG
1	G	442	ARG
1	G	475	LYS
1	H	41	ASP
1	H	57	ARG
1	H	81	THR
1	H	90	ARG
1	H	105	GLN
1	H	115	GLN
1	H	116	GLN
1	H	124	GLN
1	H	145	SER
1	H	152	ARG
1	H	168	LYS
1	H	177	GLU
1	H	225	MET
1	H	228	LYS
1	H	277	THR
1	H	295	GLN
1	H	301	VAL
1	H	302	GLU
1	H	308	ILE
1	H	310	ARG
1	H	321	HIS
1	H	342	LEU
1	H	344	SER
1	H	365	GLU
1	H	373	GLU
1	H	375	LEU
1	H	378	LEU
1	H	388	GLU
1	H	421	ASN
1	H	442	ARG
1	H	458	LEU
1	H	471	SER

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Mol	Chain	Res	Type
1	H	488	GLN
1	H	490	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
1	A	223	ASN
1	A	345	GLN
1	A	372	ASN
1	A	386	GLN
1	A	421	ASN
1	A	425	GLN
1	A	426	ASN
1	B	116	GLN
1	B	165	GLN
1	B	421	ASN
1	B	425	GLN
1	B	426	ASN
1	B	488	GLN
1	C	223	ASN
1	C	386	GLN
1	C	421	ASN
1	C	425	GLN
1	C	426	ASN
1	D	165	GLN
1	D	266	GLN
1	D	421	ASN
1	D	425	GLN
1	D	426	ASN
1	E	165	GLN
1	E	266	GLN
1	E	343	ASN
1	E	421	ASN
1	E	425	GLN
1	E	426	ASN
1	E	488	GLN
1	F	223	ASN
1	F	372	ASN
1	F	386	GLN
1	F	421	ASN
1	F	425	GLN

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Mol	Chain	Res	Type
1	F	426	ASN
1	G	165	GLN
1	G	343	ASN
1	G	421	ASN
1	G	425	GLN
1	G	426	ASN
1	G	488	GLN
1	H	223	ASN
1	H	386	GLN
1	H	395	GLN
1	H	421	ASN
1	H	425	GLN
1	H	426	ASN
1	H	490	ASN

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

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	0OR	B	501[A]	-	17,22,22	0.50	0	26,33,33	1.68	3 (11%)
2	0OR	D	501[A]	-	17,22,22	0.54	0	26,33,33	1.66	3 (11%)
2	0OR	E	501[A]	-	17,22,22	0.50	0	26,33,33	1.69	3 (11%)
2	0OR	G	501[A]	-	17,22,22	0.53	0	26,33,33	1.62	3 (11%)

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
2	0OR	B	501[A]	-	-	0/29/29/29	0/0/0/0
2	0OR	D	501[A]	-	-	0/29/29/29	0/0/0/0
2	0OR	E	501[A]	-	-	0/29/29/29	0/0/0/0
2	0OR	G	501[A]	-	-	0/29/29/29	0/0/0/0

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	501[A]	0OR	P24-O23-P20	-3.64	120.45	132.67
2	G	501[A]	0OR	P24-O23-P20	-3.57	120.70	132.67
2	B	501[A]	0OR	P24-O23-P20	-3.47	121.02	132.67
2	D	501[A]	0OR	P24-O23-P20	-3.41	121.24	132.67
2	G	501[A]	0OR	C31-C29-C32	2.70	114.28	109.34
2	B	501[A]	0OR	C31-C29-C32	2.73	114.33	109.34
2	E	501[A]	0OR	C31-C29-C32	2.84	114.54	109.34
2	D	501[A]	0OR	C31-C29-C32	2.86	114.56	109.34
2	G	501[A]	0OR	C37-N36-C34	5.58	133.57	122.53
2	D	501[A]	0OR	C37-N36-C34	5.59	133.60	122.53
2	E	501[A]	0OR	C37-N36-C34	5.78	133.96	122.53
2	B	501[A]	0OR	C37-N36-C34	5.85	134.11	122.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501[A]	0OR	2	0
2	D	501[A]	0OR	2	0
2	E	501[A]	0OR	2	0
2	G	501[A]	0OR	4	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, 95^{th} 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	456/458 (99%)	0.23	5 (1%)	82 78	40, 43, 45, 46	0
1	B	440/458 (96%)	0.28	6 (1%)	78 73	40, 44, 46, 47	0
1	C	446/458 (97%)	0.25	11 (2%)	61 54	40, 44, 46, 48	0
1	D	445/458 (97%)	0.19	4 (0%)	85 82	40, 43, 45, 73	0
1	E	439/458 (95%)	0.37	7 (1%)	74 69	41, 44, 46, 47	0
1	F	449/458 (98%)	0.25	5 (1%)	82 78	40, 43, 45, 48	0
1	G	442/458 (96%)	0.19	5 (1%)	82 78	39, 43, 45, 48	0
1	H	446/458 (97%)	0.18	2 (0%)	93 92	40, 43, 45, 47	0
All	All	3563/3664 (97%)	0.24	45 (1%)	79 74	39, 44, 46, 73	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	64	ALA	6.5
1	G	217	ALA	3.9
1	B	386	GLN	3.7
1	D	64	ALA	3.4
1	C	217	ALA	3.4
1	F	114	GLN	3.4
1	C	414	TYR	3.3
1	G	53	ALA	3.2
1	A	350	GLY	3.1
1	E	281	ASN	2.9
1	E	445	THR	2.7
1	A	367	THR	2.7
1	A	372	ASN	2.7
1	F	103	ALA	2.7
1	E	66	GLY	2.6
1	B	282	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	429	VAL	2.6
1	H	393	ALA	2.5
1	B	64	ALA	2.5
1	B	58	GLU	2.5
1	F	372	ASN	2.5
1	E	386	GLN	2.5
1	H	274	PRO	2.4
1	G	274	PRO	2.4
1	D	491	SER	2.4
1	C	352	ASN	2.3
1	C	274	PRO	2.3
1	E	478	GLU	2.3
1	D	276	GLU	2.3
1	C	275	SER	2.2
1	B	427	GLY	2.2
1	F	119	ALA	2.2
1	D	116	GLN	2.1
1	C	221	VAL	2.1
1	C	321	HIS	2.1
1	A	398	LEU	2.1
1	E	217	ALA	2.1
1	G	64	ALA	2.1
1	A	81	THR	2.1
1	F	179	ASN	2.1
1	C	411	HIS	2.0
1	G	106	SER	2.0
1	C	285	ALA	2.0
1	B	283	ILE	2.0
1	C	47	ALA	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

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, 95^{th} 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(Å^2)	Q<0.9
2	0OR	B	501[A]	23/23	0.60	0.55	5.57	75,76,76,76	23
2	0OR	D	501[A]	23/23	0.67	0.52	4.97	75,76,76,76	23
2	0OR	E	501[A]	23/23	0.63	0.55	4.56	75,76,76,76	23
2	0OR	G	501[A]	23/23	0.78	0.44	3.27	74,76,76,76	23

6.5 Other polymers

There are no such residues in this entry.