Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 03:07 PM EDT

PDB ID	:	5E1R
Title	:	Crystal structure of pecan (carya illinoinensis) vicilin, a new food allergen
Authors	:	Zhang, Y.Z.
Deposited on	:	2015-09-30
Resolution	:	2.65 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 (1)) were used in the production of this report:

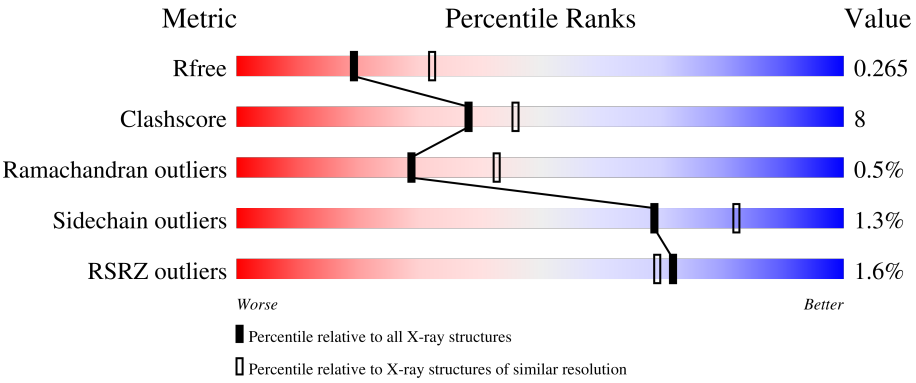
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	426	68% 15% 16%
1	B	426	2% 67% 15% 17%
1	C	426	% 66% 17% 16%
1	D	426	2% 68% 15% 16%
1	E	426	% 69% 14% 16%

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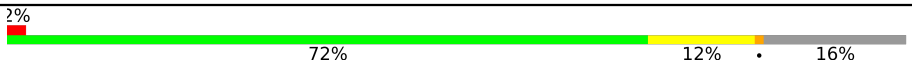
Mol	Chain	Length	Quality of chain
1	F	426	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17082 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 7S vicilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	1	0
			2841	1789	504	539	9			
1	B	355	Total	C	N	O	S	0	0	0
			2799	1766	490	534	9			
1	C	358	Total	C	N	O	S	0	0	0
			2826	1785	499	533	9			
1	D	357	Total	C	N	O	S	0	0	0
			2838	1785	508	536	9			
1	E	358	Total	C	N	O	S	0	0	0
			2866	1799	512	546	9			
1	F	358	Total	C	N	O	S	0	0	0
			2818	1776	496	537	9			

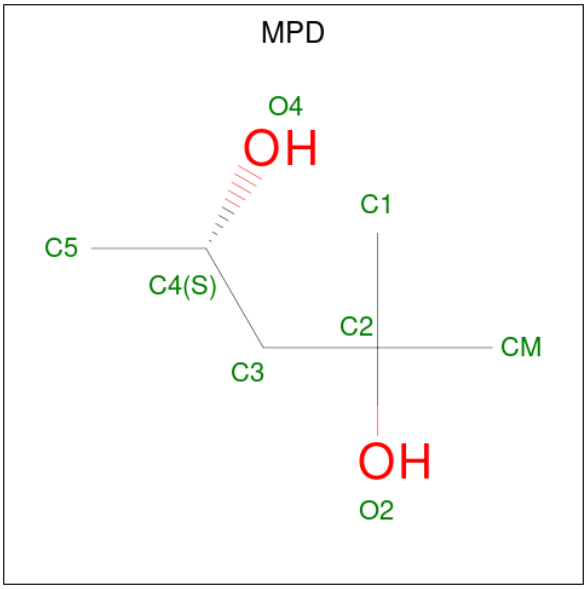
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	367	MET	-	initiating methionine	UNP B3STU4
A	368	SER	-	expression tag	UNP B3STU4
B	367	MET	-	initiating methionine	UNP B3STU4
B	368	SER	-	expression tag	UNP B3STU4
C	367	MET	-	initiating methionine	UNP B3STU4
C	368	SER	-	expression tag	UNP B3STU4
D	367	MET	-	initiating methionine	UNP B3STU4
D	368	SER	-	expression tag	UNP B3STU4
E	367	MET	-	initiating methionine	UNP B3STU4
E	368	SER	-	expression tag	UNP B3STU4
F	367	MET	-	initiating methionine	UNP B3STU4
F	368	SER	-	expression tag	UNP B3STU4

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cu 1 1	0	0
2	B	1	Total Cu 1 1	0	0
2	C	1	Total Cu 1 1	0	0
2	D	1	Total Cu 1 1	0	0
2	E	1	Total Cu 1 1	0	0
2	F	1	Total Cu 1 1	0	0

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	C	1	Total C O 8 6 2	0	0
3	D	1	Total C O 8 6 2	0	0
3	E	1	Total C O 8 6 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C O 8 6 2	0	0

- Molecule 4 is water.

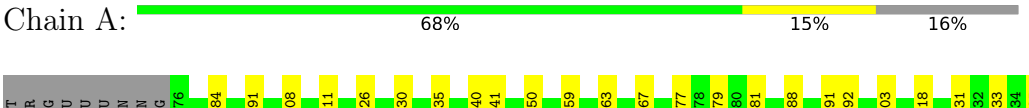
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	7	Total O 7 7	0	0
4	B	8	Total O 8 8	0	0
4	C	7	Total O 7 7	0	0
4	D	7	Total O 7 7	0	0
4	E	8	Total O 8 8	0	0
4	F	3	Total O 3 3	0	0

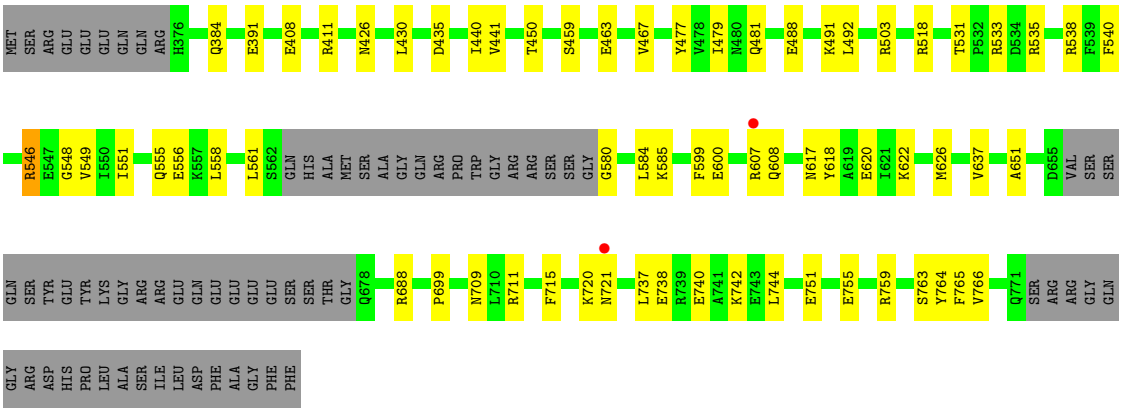
3 Residue-property plots (i)

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: 7S vicilin

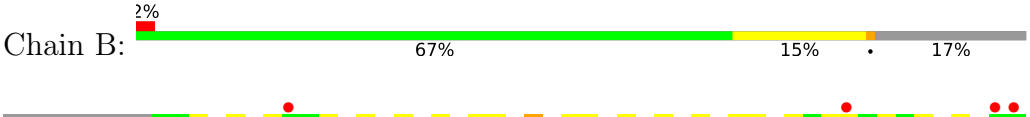
Chain A:

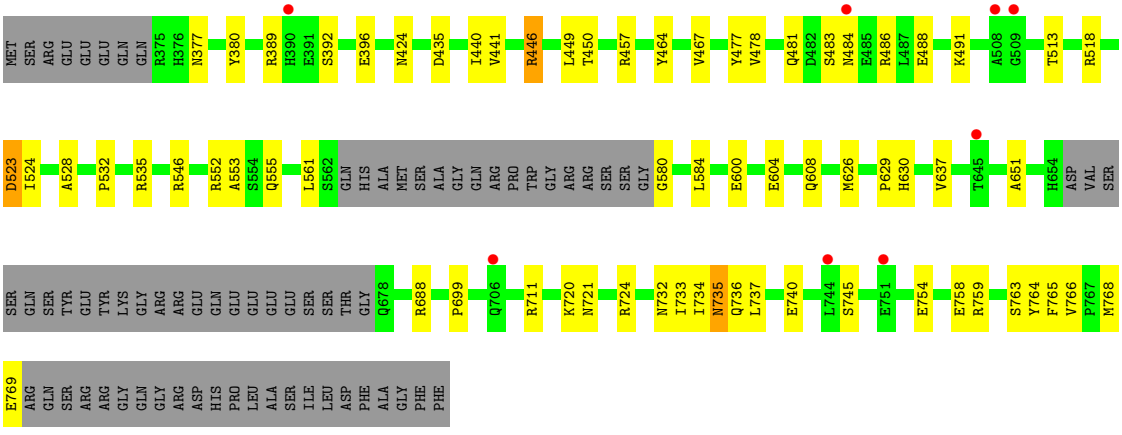




- Molecule 1: 7S vicilin

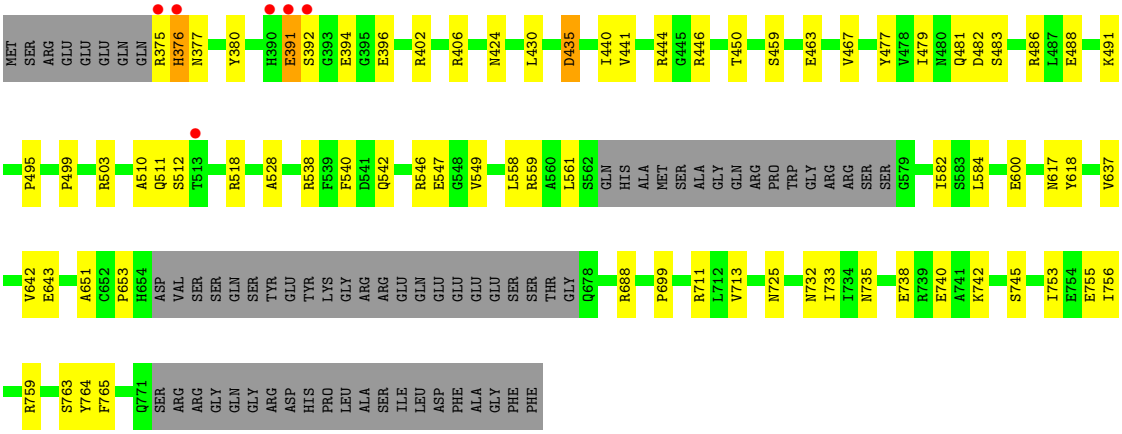
Chain B:





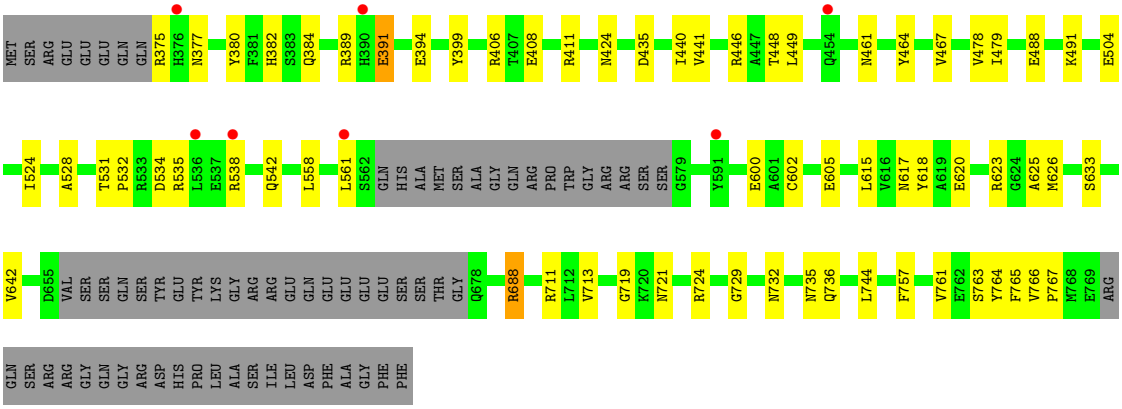
- Molecule 1: 7S vicilin

Chain C:



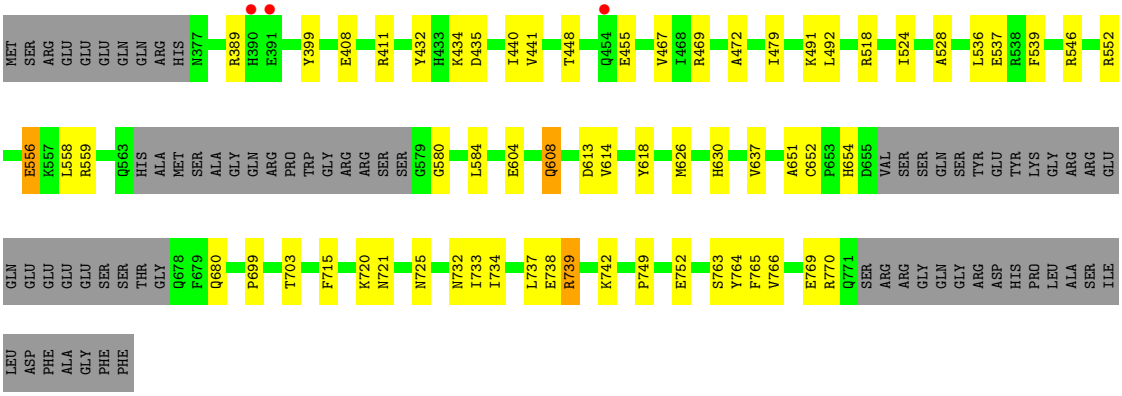
• Molecule 1: 7S vicilin

Chain D:



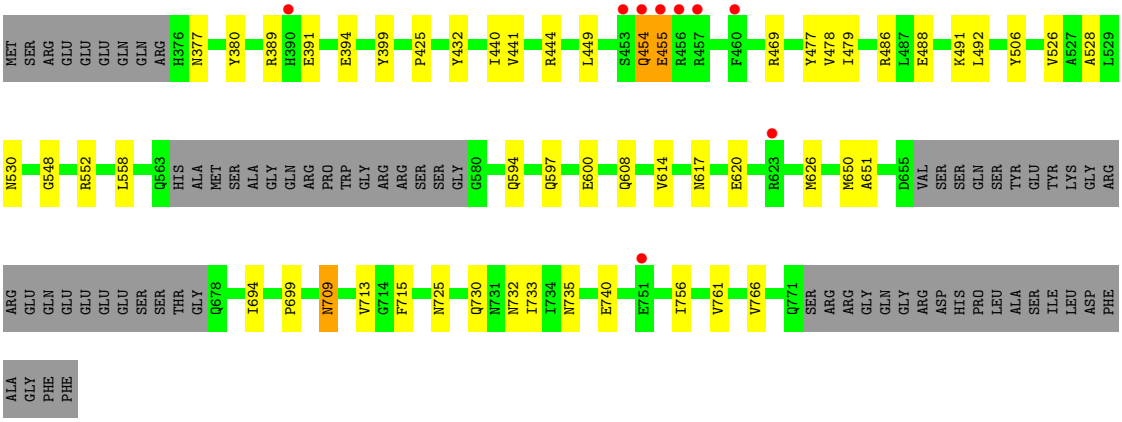
• Molecule 1: 7S vicilin

Chain E:



• Molecule 1: 7S vicilin

Chain F:


MET SER ARG GLU GLU GLU GLN GLN ARG H376 N377 Y380 R389 H390 E391 E394 Y399 P425 Y432 I440 V441 R444 L449 S453 Q454 E455 R456 R457 F460 R469 Y477 V478 I479 R486 L487 E488 K491 L492 Y506 V526 A527 A528 L529
N530 G548 R552 L558 Q563 HIS ALA MET SER ALA GLY GLN ARG PRO TRP GLY ARG ARG SER SER GLY G580 Q594 Q597 E600 Q608 V614 N617 E620 R623 M626 M650 A651 D655 VAL SER SER GLN SER TYR GLU TYR LYS GLY ARG
ARG GLU GLN GLU GLU GLU GLU SER SER THR GLY Q678 I694 P699 N709 V713 G714 F715 N725 Q730 N731 N732 I733 I734 N735 E740 E751 I756 V761 V766 Q771 SER ARG ARG GLY GLN GLY ARG ASP HIS PRO LEU ALA SER ILE LEU ASP PHE
ALA GLY PHE PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	42.69Å 151.61Å 342.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.60 – 2.65 48.47 – 2.65	Depositor EDS
% Data completeness (in resolution range)	89.0 (46.60-2.65) 89.1 (48.47-2.65)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.65Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.218 , 0.262 0.225 , 0.265	Depositor DCC
R_{free} test set	2000 reflections (3.38%)	wwPDB-VP
Wilson B-factor (Å^2)	43.8	Xtriage
Anisotropy	1.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 26.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	17082	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU, MPD

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	0.27	0/2896	0.44	0/3913
1	B	0.24	0/2851	0.44	0/3856
1	C	0.25	0/2881	0.45	0/3895
1	D	0.27	0/2893	0.43	0/3911
1	E	0.26	0/2919	0.46	0/3942
1	F	0.24	0/2872	0.44	0/3887
All	All	0.26	0/17312	0.44	0/23404

There are no bond length outliers.

There are no bond angle outliers.

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	2841	0	2741	53	0
1	B	2799	0	2684	57	0
1	C	2826	0	2707	53	0
1	D	2838	0	2731	46	0
1	E	2866	0	2769	45	0
1	F	2818	0	2688	35	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	8	0	14	2	0
3	B	8	0	14	1	0
3	C	8	0	14	1	0
3	D	8	0	14	1	0
3	E	8	0	14	2	0
3	F	8	0	14	0	0
4	A	7	0	0	0	0
4	B	8	0	0	0	0
4	C	7	0	0	0	0
4	D	7	0	0	0	0
4	E	8	0	0	0	0
4	F	3	0	0	0	0
All	All	17082	0	16404	254	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 8.

All (254) 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:709:ASN:HD22	1:F:709:ASN:H	1.20	0.90
1:E:720:LYS:HG2	1:E:721:ASN:HD22	1.40	0.87
1:B:532:PRO:HG2	1:B:535:ARG:HD3	1.60	0.83
1:B:735:ASN:N	1:B:735:ASN:HD22	1.76	0.83
1:B:389:ARG:NH2	1:B:513:THR:OG1	2.15	0.80
1:B:457:ARG:NH2	1:B:477:TYR:OH	2.15	0.79
1:C:375:ARG:HH11	1:C:377:ASN:HB2	1.48	0.78
1:D:744:LEU:O	1:E:546:ARG:NH1	2.18	0.77
1:C:394:GLU:OE1	1:C:424:ASN:ND2	2.18	0.76
1:C:642:VAL:HB	1:C:711:ARG:HG2	1.67	0.76
1:F:709:ASN:HD22	1:F:709:ASN:N	1.82	0.76
1:C:732:ASN:HD21	1:C:735:ASN:ND2	1.84	0.75
1:B:732:ASN:OD1	1:B:734:ILE:N	2.20	0.75
1:D:642:VAL:O	1:D:688:ARG:NH1	2.22	0.73
1:F:651:ALA:HB3	1:F:699:PRO:HG2	1.70	0.72
1:A:763:SER:O	1:A:765:PHE:N	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ASN:HA	1:B:486:ARG:HG2	1.72	0.72
1:C:424:ASN:OD1	1:C:486:ARG:NH1	2.23	0.71
1:B:651:ALA:HB3	1:B:699:PRO:HG2	1.72	0.71
1:C:651:ALA:HB3	1:C:699:PRO:HG2	1.72	0.70
1:B:769:GLU:OE2	1:D:446:ARG:NH2	2.24	0.70
1:D:763:SER:O	1:D:765:PHE:N	2.24	0.70
1:A:580:GLY:O	1:A:608:GLN:NE2	2.23	0.69
1:E:440:ILE:HG12	1:E:491:LYS:HG2	1.73	0.69
1:A:755:GLU:OE1	1:B:535:ARG:NH2	2.26	0.68
1:A:488:GLU:OE1	1:A:688:ARG:NH2	2.27	0.68
1:B:424:ASN:OD1	1:B:486:ARG:NH1	2.27	0.68
1:B:440:ILE:HG12	1:B:491:LYS:HG2	1.75	0.68
1:A:755:GLU:HB3	1:B:535:ARG:HH21	1.58	0.67
1:A:651:ALA:HB3	1:A:699:PRO:HG2	1.77	0.67
1:C:763:SER:O	1:C:765:PHE:N	2.28	0.67
1:A:535:ARG:HG2	1:A:538:ARG:HH22	1.60	0.66
1:F:425:PRO:HD3	1:F:486:ARG:HG2	1.77	0.66
1:C:643:GLU:OE1	1:C:711:ARG:NH1	2.29	0.65
1:D:735:ASN:ND2	1:D:757:PHE:O	2.30	0.65
1:D:729:GLY:O	1:D:732:ASN:ND2	2.26	0.65
1:E:651:ALA:HB3	1:E:699:PRO:HG2	1.79	0.65
1:E:720:LYS:HG2	1:E:721:ASN:ND2	2.10	0.65
1:A:751:GLU:O	1:A:755:GLU:HG2	1.97	0.64
1:E:766:VAL:HG21	1:F:528:ALA:HA	1.79	0.64
1:F:440:ILE:HG12	1:F:491:LYS:HG2	1.80	0.64
1:F:597:GLN:NE2	1:F:620:GLU:OE2	2.24	0.64
1:A:738:GLU:H	1:B:457:ARG:HH12	1.46	0.64
1:C:440:ILE:HG12	1:C:491:LYS:HG2	1.78	0.63
1:A:440:ILE:HG12	1:A:491:LYS:HG2	1.80	0.63
1:D:408:GLU:HG3	1:D:411:ARG:HD3	1.79	0.63
1:E:770:ARG:HD3	1:F:530:ASN:HA	1.81	0.62
1:F:389:ARG:HB2	1:F:399:TYR:HE2	1.65	0.62
1:B:552:ARG:NH1	1:B:553:ALA:O	2.33	0.62
1:D:488:GLU:OE2	1:D:688:ARG:NH2	2.32	0.62
1:E:556:GLU:HG3	1:E:559:ARG:HH21	1.64	0.62
1:C:441:VAL:HG11	1:C:713:VAL:HG21	1.82	0.62
1:F:732:ASN:ND2	1:F:735:ASN:OD1	2.33	0.62
1:A:408:GLU:OE1	1:A:411:ARG:NH2	2.33	0.62
1:E:626:MET:HB2	1:E:703:THR:HG22	1.82	0.61
1:B:464:TYR:OH	1:B:711:ARG:NH2	2.33	0.61
1:D:732:ASN:HD21	1:D:735:ASN:ND2	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:637:VAL:HG11	3:E:802:MPD:H52	1.81	0.61
1:D:464:TYR:OH	1:D:711:ARG:NH1	2.34	0.61
1:D:440:ILE:HG12	1:D:491:LYS:HG2	1.83	0.61
1:D:602:CYS:HA	1:D:615:LEU:HD23	1.81	0.61
1:F:441:VAL:HG11	1:F:713:VAL:HG21	1.81	0.61
1:C:375:ARG:HA	1:C:376:HIS:ND1	2.16	0.61
1:B:392:SER:HB3	1:B:396:GLU:HA	1.81	0.61
1:D:389:ARG:HB2	1:D:399:TYR:HE1	1.66	0.60
1:E:654:HIS:O	1:E:680:GLN:NE2	2.34	0.60
1:A:518:ARG:HD2	1:A:540:PHE:CG	2.36	0.59
1:C:377:ASN:HB3	1:C:380:TYR:HB3	1.84	0.59
1:B:735:ASN:N	1:B:735:ASN:ND2	2.49	0.58
1:C:375:ARG:NH1	1:C:377:ASN:HB2	2.16	0.58
1:B:763:SER:O	1:B:765:PHE:N	2.36	0.58
1:A:535:ARG:HA	1:A:538:ARG:NH2	2.19	0.58
1:A:720:LYS:HG2	1:A:721:ASN:HD22	1.69	0.57
1:B:446:ARG:HH21	1:B:481:GLN:HG3	1.69	0.57
1:C:380:TYR:O	1:C:406:ARG:NH2	2.27	0.57
1:C:479:ILE:HG23	1:C:558:LEU:HD22	1.86	0.57
1:C:732:ASN:ND2	1:C:735:ASN:HD22	2.03	0.57
1:D:441:VAL:HG11	1:D:713:VAL:HG21	1.85	0.57
1:C:584:LEU:HD13	1:C:618:TYR:HB2	1.86	0.57
1:D:617:ASN:OD1	3:D:802:MPD:O2	2.22	0.57
1:B:377:ASN:HB3	1:B:380:TYR:HB3	1.87	0.57
1:E:432:TYR:HE2	1:E:434:LYS:HE3	1.70	0.56
1:E:769:GLU:OE1	1:E:769:GLU:N	2.38	0.56
1:B:732:ASN:O	1:B:736:GLN:NE2	2.29	0.56
1:E:732:ASN:OD1	1:E:734:ILE:N	2.37	0.56
1:D:766:VAL:HG21	1:E:528:ALA:HA	1.87	0.56
1:B:745:SER:O	1:C:546:ARG:NH2	2.37	0.55
1:C:446:ARG:NH2	1:C:463:GLU:OE1	2.40	0.55
1:E:479:ILE:HG23	1:E:558:LEU:HD22	1.87	0.55
1:A:546[A]:ARG:HB3	1:A:546[A]:ARG:NH1	2.21	0.55
1:F:709:ASN:N	1:F:709:ASN:ND2	2.50	0.55
1:F:454:GLN:HG2	1:F:455:GLU:N	2.21	0.55
1:C:467:VAL:HB	1:C:582:ILE:HB	1.88	0.54
1:D:531:THR:HG21	1:F:756:ILE:HG23	1.89	0.54
1:A:441:VAL:HG22	1:A:467:VAL:HG22	1.90	0.54
1:E:518:ARG:NH2	1:E:537:GLU:OE1	2.41	0.54
1:E:556:GLU:HG3	1:E:559:ARG:NH2	2.23	0.54
1:D:479:ILE:HG23	1:D:558:LEU:HD22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:GLU:OE2	1:B:724:ARG:NH2	2.34	0.53
1:B:637:VAL:HG11	3:B:802:MPD:H52	1.90	0.53
1:D:732:ASN:CG	1:D:735:ASN:HD22	2.10	0.53
1:C:732:ASN:CG	1:C:735:ASN:HD22	2.11	0.53
1:C:755:GLU:OE2	1:C:759:ARG:NH2	2.38	0.53
1:A:535:ARG:HA	1:A:538:ARG:HH21	1.74	0.53
1:A:435:ASP:OD1	1:A:435:ASP:N	2.36	0.53
1:C:511:GLN:HB2	1:C:547:GLU:OE1	2.08	0.53
1:F:444:ARG:HE	1:F:488:GLU:HB2	1.73	0.53
1:A:479:ILE:HG23	1:A:558:LEU:HD22	1.91	0.53
1:A:755:GLU:HB3	1:B:535:ARG:NH2	2.21	0.53
1:B:389:ARG:O	1:B:392:SER:OG	2.26	0.52
1:D:408:GLU:HG3	1:D:411:ARG:CD	2.39	0.52
1:D:449:LEU:HD12	1:D:478:VAL:HG22	1.92	0.52
1:C:402:ARG:NH2	1:C:499:PRO:O	2.43	0.51
1:F:492:LEU:HD22	1:F:715:PHE:HB3	1.93	0.51
1:B:483:SER:OG	1:B:555:GLN:NE2	2.37	0.51
1:B:754:GLU:O	1:B:759:ARG:NH1	2.43	0.51
1:A:738:GLU:N	1:B:457:ARG:HH12	2.08	0.51
1:B:735:ASN:HD22	1:B:735:ASN:H	1.55	0.51
1:D:389:ARG:NH1	1:D:504:GLU:OE1	2.43	0.51
1:A:492:LEU:HD22	1:A:715:PHE:HB3	1.92	0.51
1:E:725:ASN:HB3	1:E:733:ILE:HG21	1.93	0.51
1:A:391:GLU:O	1:A:548:GLY:HA2	2.11	0.51
1:F:449:LEU:HD12	1:F:478:VAL:HG22	1.92	0.51
1:B:740:GLU:HB2	1:C:561:LEU:HD21	1.93	0.50
1:A:546[A]:ARG:HH21	1:A:551:ILE:HD12	1.75	0.50
1:B:626:MET:HE3	1:B:629:PRO:HD3	1.92	0.50
1:E:441:VAL:HG22	1:E:467:VAL:HG22	1.94	0.50
1:E:738:GLU:OE2	1:F:477:TYR:OH	2.30	0.50
1:F:394:GLU:HG3	1:F:552:ARG:HG2	1.93	0.50
1:A:477:TYR:OH	1:C:738:GLU:OE1	2.28	0.50
1:C:450:THR:HG1	1:C:459:SER:HG	1.58	0.50
1:E:763:SER:O	1:E:765:PHE:N	2.42	0.49
1:C:637:VAL:HG11	3:C:802:MPD:H31	1.94	0.49
1:D:448:THR:OG1	1:D:461:ASN:OD1	2.20	0.49
1:A:384:GLN:N	1:A:384:GLN:OE1	2.45	0.49
1:A:426:ASN:ND2	1:A:555:GLN:OE1	2.32	0.49
1:D:615:LEU:HG	1:D:719:GLY:HA3	1.95	0.49
1:A:737:LEU:HA	1:B:457:ARG:NH1	2.27	0.49
1:B:737:LEU:HD22	1:C:477:TYR:HE2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:448:THR:HB	1:E:479:ILE:HB	1.95	0.48
1:A:622:LYS:HD2	1:A:709:ASN:HD21	1.79	0.48
1:D:382:HIS:CE1	1:D:384:GLN:HG3	2.48	0.48
1:E:492:LEU:HD22	1:E:715:PHE:HB3	1.95	0.48
1:E:770:ARG:CD	1:F:530:ASN:HA	2.44	0.48
1:F:444:ARG:HH21	1:F:488:GLU:HB2	1.79	0.48
1:D:626:MET:HE1	1:E:524:ILE:HG23	1.97	0.47
1:B:720:LYS:HB3	1:B:720:LYS:HE3	1.63	0.47
1:A:759:ARG:HA	1:A:759:ARG:HD3	1.59	0.47
1:D:561:LEU:HD21	1:F:740:GLU:HB2	1.97	0.47
1:C:488:GLU:OE1	1:C:688:ARG:NH2	2.48	0.47
1:D:736:GLN:NE2	1:E:455:GLU:O	2.48	0.47
1:E:432:TYR:CE2	1:E:434:LYS:HE3	2.50	0.47
1:E:739:ARG:H	1:E:739:ARG:HG2	1.50	0.47
1:E:770:ARG:NH2	1:F:526:VAL:O	2.48	0.47
1:A:740:GLU:HB2	1:B:561:LEU:HD21	1.96	0.47
1:B:450:THR:HG21	1:B:457:ARG:NH2	2.30	0.47
1:E:580:GLY:O	1:E:608:GLN:NE2	2.48	0.47
1:D:382:HIS:HE1	1:D:384:GLN:HG3	1.80	0.46
1:D:618:TYR:OH	1:D:711:ARG:HD2	2.15	0.46
1:E:389:ARG:HB2	1:E:399:TYR:HE1	1.81	0.46
1:A:450:THR:HG1	1:A:459:SER:HG	1.62	0.46
1:B:580:GLY:O	1:B:608:GLN:NE2	2.38	0.46
1:E:604:GLU:OE2	1:E:721:ASN:N	2.35	0.46
1:B:484:ASN:OD1	1:B:484:ASN:N	2.48	0.46
1:B:766:VAL:HG21	1:C:528:ALA:HA	1.98	0.46
1:A:637:VAL:HG11	3:A:802:MPD:H31	1.97	0.46
1:B:758:GLU:HB2	1:B:759:ARG:NH1	2.30	0.46
1:A:585:LYS:HA	1:A:599:PHE:CD1	2.50	0.46
1:C:538:ARG:O	1:C:542:GLN:HG2	2.15	0.46
1:E:408:GLU:OE2	1:E:411:ARG:NH2	2.42	0.46
1:A:766:VAL:HG21	1:B:528:ALA:HA	1.96	0.46
1:F:730:GLN:OE1	1:F:761:VAL:HA	2.16	0.46
1:C:435:ASP:OD2	1:C:503:ARG:N	2.46	0.46
1:B:435:ASP:OD1	1:B:435:ASP:N	2.42	0.45
1:A:626:MET:HE1	1:B:524:ILE:HG23	1.98	0.45
1:A:755:GLU:OE2	1:A:759:ARG:NH2	2.45	0.45
1:E:613:ASP:OD1	1:E:720:LYS:HB2	2.16	0.45
1:B:450:THR:HG21	1:B:457:ARG:HH21	1.82	0.45
1:F:479:ILE:HG23	1:F:558:LEU:HD22	1.98	0.45
1:A:518:ARG:HD2	1:A:540:PHE:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:584:LEU:HD13	1:E:618:TYR:HB2	1.98	0.45
1:A:463:GLU:N	1:A:463:GLU:OE1	2.50	0.45
1:C:391:GLU:OE2	1:C:549:VAL:HG13	2.16	0.45
1:D:441:VAL:HG22	1:D:467:VAL:HG22	1.98	0.45
1:C:481:GLN:HE21	1:C:559:ARG:HA	1.82	0.45
1:D:524:ILE:HG23	1:F:626:MET:HE1	1.99	0.45
1:D:732:ASN:ND2	1:D:735:ASN:HD22	2.15	0.45
1:B:446:ARG:NH2	1:B:481:GLN:HG3	2.31	0.44
1:D:732:ASN:ND2	1:D:735:ASN:ND2	2.64	0.44
1:E:737:LEU:O	1:E:742:LYS:HE3	2.17	0.44
1:C:450:THR:OG1	1:C:459:SER:OG	2.32	0.44
1:D:620:GLU:HG3	1:D:711:ARG:HG2	1.98	0.44
1:A:737:LEU:HB2	1:A:742:LYS:HG3	1.98	0.44
1:A:384:GLN:H	1:A:384:GLN:CD	2.20	0.44
1:B:449:LEU:HD12	1:B:478:VAL:HG22	1.99	0.44
1:B:604:GLU:OE2	1:B:721:ASN:N	2.37	0.44
1:E:749:PRO:HG2	1:E:752:GLU:HG3	1.99	0.44
1:A:620:GLU:HG3	1:A:711:ARG:HG2	2.00	0.44
1:C:518:ARG:HD3	1:C:540:PHE:CD2	2.53	0.44
1:A:546[B]:ARG:NH1	1:C:745:SER:O	2.50	0.44
1:A:430:LEU:HD12	1:A:549:VAL:HA	2.00	0.43
1:A:600:GLU:HG3	1:A:617:ASN:HB3	2.01	0.43
1:B:626:MET:HE1	1:C:528:ALA:HB2	1.99	0.43
1:D:625:ALA:HA	1:D:767:PRO:HA	1.99	0.43
1:A:584:LEU:HD13	1:A:618:TYR:HB2	1.99	0.43
1:B:732:ASN:OD1	1:B:733:ILE:N	2.51	0.43
1:D:535:ARG:HG2	1:D:538:ARG:NH2	2.33	0.43
1:E:732:ASN:OD1	1:E:733:ILE:N	2.52	0.43
1:A:561:LEU:HD21	1:C:740:GLU:HB2	1.99	0.43
1:B:441:VAL:HG22	1:B:467:VAL:HG22	2.01	0.43
1:C:430:LEU:HD12	1:C:549:VAL:HA	2.01	0.43
1:E:435:ASP:OD1	1:E:435:ASP:N	2.41	0.43
1:A:503:ARG:HG3	1:C:653:PRO:HG2	1.99	0.43
1:D:380:TYR:O	1:D:406:ARG:NH2	2.50	0.43
1:F:469:ARG:HB3	1:F:608:GLN:HG3	2.01	0.43
1:F:377:ASN:HB3	1:F:380:TYR:HB3	2.00	0.43
1:B:518:ARG:O	1:B:518:ARG:HG3	2.19	0.42
1:B:584:LEU:HD12	1:B:584:LEU:HA	1.87	0.42
1:C:732:ASN:ND2	1:C:735:ASN:ND2	2.54	0.42
1:E:469:ARG:N	1:E:608:GLN:OE1	2.42	0.42
1:F:444:ARG:HB3	1:F:488:GLU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:SER:HB3	1:C:396:GLU:HA	2.01	0.42
1:D:532:PRO:HB2	1:D:534:ASP:OD1	2.19	0.42
1:F:391:GLU:O	1:F:548:GLY:HA2	2.19	0.42
1:D:377:ASN:HB3	1:D:380:TYR:HB3	2.00	0.42
1:A:637:VAL:HG21	3:A:802:MPD:H52	2.01	0.42
1:B:488:GLU:OE1	1:B:688:ARG:NH2	2.52	0.42
1:D:435:ASP:OD1	1:D:435:ASP:N	2.42	0.42
1:D:633:SER:HB2	1:E:472:ALA:O	2.20	0.42
1:C:725:ASN:HB3	1:C:733:ILE:HG21	2.01	0.42
1:F:432:TYR:HB3	1:F:506:TYR:CD1	2.55	0.42
1:C:435:ASP:O	1:C:495:PRO:HA	2.20	0.41
1:F:600:GLU:HG3	1:F:617:ASN:HB3	2.03	0.41
1:A:744:LEU:O	1:B:546:ARG:NH1	2.46	0.41
1:B:630:HIS:O	1:B:699:PRO:HA	2.20	0.41
1:F:725:ASN:HB3	1:F:733:ILE:HG21	2.02	0.41
1:A:556:GLU:H	1:A:556:GLU:HG3	1.73	0.41
1:D:600:GLU:OE2	1:D:724:ARG:NH2	2.40	0.41
1:A:481:GLN:O	1:A:555:GLN:NE2	2.53	0.41
1:A:531:THR:HG21	1:C:756:ILE:HD13	2.01	0.41
1:C:742:LYS:HB3	1:C:753:ILE:HD13	2.03	0.41
1:D:394:GLU:HG3	1:D:424:ASN:HD22	1.86	0.41
1:E:630:HIS:HE1	3:E:802:MPD:O4	2.04	0.41
1:C:510:ALA:C	1:C:512:SER:H	2.24	0.41
1:E:652:CYS:O	1:E:680:GLN:HG3	2.21	0.41
1:F:650:MET:HE1	1:F:694:ILE:HA	2.03	0.40
1:D:375:ARG:HD3	1:D:375:ARG:HA	1.80	0.40
1:B:523:ASP:OD1	1:B:523:ASP:N	2.54	0.40
1:C:482:ASP:OD1	1:C:483:SER:N	2.55	0.40
1:C:600:GLU:HG3	1:C:617:ASN:HB3	2.02	0.40
1:C:759:ARG:HA	1:C:759:ARG:HD3	1.85	0.40
1:E:536:LEU:O	1:E:539:PHE:HB3	2.22	0.40
1:C:444:ARG:HH12	1:C:688:ARG:NH2	2.19	0.40
1:D:528:ALA:HA	1:F:766:VAL:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	352/426 (83%)	336 (96%)	15 (4%)	1 (0%)	41	56
1	B	349/426 (82%)	333 (95%)	14 (4%)	2 (1%)	25	37
1	C	352/426 (83%)	334 (95%)	17 (5%)	1 (0%)	41	56
1	D	351/426 (82%)	332 (95%)	16 (5%)	3 (1%)	17	26
1	E	352/426 (83%)	335 (95%)	16 (4%)	1 (0%)	41	56
1	F	352/426 (83%)	332 (94%)	18 (5%)	2 (1%)	25	37
All	All	2108/2556 (82%)	2002 (95%)	96 (5%)	10 (0%)	29	43

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	764	TYR
1	C	764	TYR
1	D	721	ASN
1	D	764	TYR
1	B	764	TYR
1	D	391	GLU
1	B	768	MET
1	E	764	TYR
1	F	454	GLN
1	F	455	GLU

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	298/369 (81%)	294 (99%)	4 (1%)	69	82
1	B	292/369 (79%)	289 (99%)	3 (1%)	76	86
1	C	293/369 (79%)	290 (99%)	3 (1%)	76	86
1	D	299/369 (81%)	293 (98%)	6 (2%)	55	73
1	E	304/369 (82%)	299 (98%)	5 (2%)	62	78
1	F	294/369 (80%)	291 (99%)	3 (1%)	76	86
All	All	1780/2214 (80%)	1756 (99%)	24 (1%)	69	82

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	533	ARG
1	A	546[A]	ARG
1	A	546[B]	ARG
1	A	607	ARG
1	B	446	ARG
1	B	523	ASP
1	B	735	ASN
1	C	376	HIS
1	C	391	GLU
1	C	435	ASP
1	D	391	GLU
1	D	542	GLN
1	D	605	GLU
1	D	623	ARG
1	D	688	ARG
1	D	761	VAL
1	E	552	ARG
1	E	556	GLU
1	E	608	GLN
1	E	614	VAL
1	E	739	ARG
1	F	594	GLN
1	F	614	VAL
1	F	709	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	721	ASN

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Mol	Chain	Res	Type
1	B	735	ASN
1	C	735	ASN
1	E	630	HIS
1	E	680	GLN
1	E	721	ASN
1	F	709	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	MPD	A	802	-	7,7,7	0.28	0	9,10,10	0.46	0
3	MPD	B	802	-	7,7,7	0.28	0	9,10,10	0.62	0
3	MPD	E	802	-	7,7,7	0.30	0	9,10,10	0.66	0
3	MPD	F	802	-	7,7,7	0.31	0	9,10,10	0.44	0
3	MPD	C	802	-	7,7,7	0.29	0	9,10,10	0.48	0
3	MPD	D	802	-	7,7,7	0.30	0	9,10,10	0.44	0

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	MPD	A	802	-	-	2/5/5/5	-
3	MPD	B	802	-	-	1/5/5/5	-
3	MPD	E	802	-	-	1/5/5/5	-
3	MPD	F	802	-	-	2/5/5/5	-
3	MPD	C	802	-	-	2/5/5/5	-
3	MPD	D	802	-	-	2/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	802	MPD	C2-C3-C4-O4
3	B	802	MPD	C2-C3-C4-C5
3	D	802	MPD	C2-C3-C4-C5
3	F	802	MPD	C2-C3-C4-C5
3	A	802	MPD	C2-C3-C4-O4
3	A	802	MPD	C2-C3-C4-C5
3	C	802	MPD	C2-C3-C4-C5
3	E	802	MPD	C2-C3-C4-C5
3	D	802	MPD	C2-C3-C4-O4
3	F	802	MPD	C2-C3-C4-O4

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	MPD	2	0
3	B	802	MPD	1	0
3	E	802	MPD	2	0
3	C	802	MPD	1	0
3	D	802	MPD	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

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	357/426 (83%)	-0.07	2 (0%)	89	89	6, 14, 29, 38	0
1	B	355/426 (83%)	0.10	8 (2%)	60	56	6, 16, 32, 42	0
1	C	358/426 (84%)	0.13	6 (1%)	70	67	6, 15, 33, 50	0
1	D	357/426 (83%)	0.05	7 (1%)	65	60	8, 18, 35, 45	0
1	E	358/426 (84%)	0.03	3 (0%)	86	85	6, 16, 31, 41	0
1	F	358/426 (84%)	0.07	9 (2%)	57	53	9, 19, 36, 48	0
All	All	2143/2556 (83%)	0.05	35 (1%)	72	69	6, 16, 33, 50	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	390	HIS	8.2
1	D	390	HIS	5.9
1	F	455	GLU	4.4
1	D	536	LEU	4.1
1	E	391	GLU	3.9
1	C	390	HIS	3.6
1	F	456	ARG	3.6
1	C	375	ARG	3.5
1	F	390	HIS	3.5
1	E	454	GLN	3.3
1	E	390	HIS	3.3
1	F	454	GLN	3.0
1	C	376	HIS	2.9
1	D	538	ARG	2.6
1	F	457	ARG	2.5
1	C	391	GLU	2.4
1	C	392	SER	2.4
1	F	460	PHE	2.3
1	D	376	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	561	LEU	2.3
1	B	744	LEU	2.2
1	B	509	GLY	2.2
1	D	591	TYR	2.2
1	A	721	ASN	2.2
1	F	453	SER	2.2
1	D	454	GLN	2.2
1	A	607	ARG	2.2
1	B	751	GLU	2.2
1	F	751	GLU	2.2
1	F	623	ARG	2.1
1	B	508	ALA	2.1
1	B	484	ASN	2.1
1	B	645	THR	2.1
1	C	513	THR	2.0
1	B	706	GLN	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, 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	B-factors(Å^2)	Q<0.9
3	MPD	D	802	8/8	0.86	0.39	9,12,15,19	0
3	MPD	F	802	8/8	0.86	0.38	12,19,25,26	0
3	MPD	A	802	8/8	0.88	0.25	8,15,19,21	0
3	MPD	B	802	8/8	0.88	0.33	6,13,20,27	0
3	MPD	E	802	8/8	0.89	0.36	10,12,21,24	0
3	MPD	C	802	8/8	0.89	0.24	4,15,21,21	0
2	CU	A	801	1/1	0.98	0.12	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CU	B	801	1/1	0.98	0.08	16,16,16,16	0
2	CU	E	801	1/1	0.99	0.07	18,18,18,18	0
2	CU	F	801	1/1	0.99	0.07	22,22,22,22	0
2	CU	C	801	1/1	0.99	0.09	11,11,11,11	0
2	CU	D	801	1/1	0.99	0.07	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.