



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 08:19 PM UTC

PDB ID : 9NSD / pdb_00009nsd
Title : Crystal structure of PvCSS-PvPTRAMP in complex with nanobody D7
Authors : Seager, B.A.; Scally, S.W.; Cowman, A.F.
Deposited on : 2025-03-16
Resolution : 3.14 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

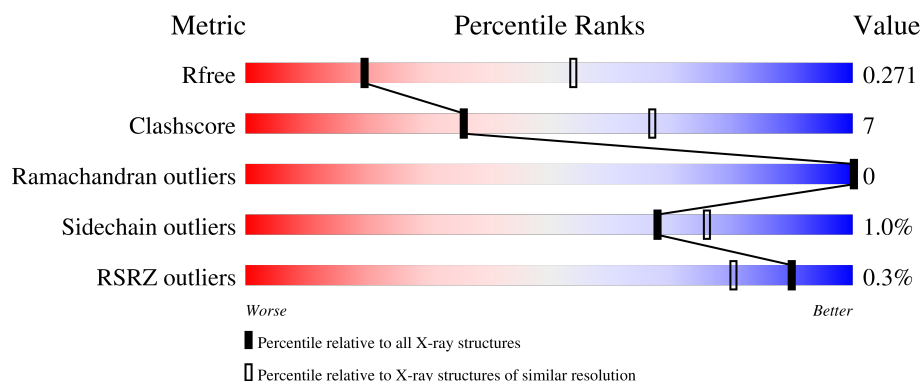
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.14 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}	180053	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	276	
1	B	276	
1	D	276	
2	C	126	
2	E	126	

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Mol	Chain	Length	Quality of chain
2	F	126	73% 23% ..
3	G	279	95% .
3	H	279	95% ..
3	I	279	96% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9548 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 Cysteine-rich small secreted protein CSS, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2153	1378	357	406	12			
1	B	264	Total	C	N	O	S	0	0	0
			2137	1369	352	404	12			
1	D	266	Total	C	N	O	S	0	0	0
			2153	1378	357	406	12			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	GLY	-	expression tag	UNP A0A565A192
A	114	THR	-	expression tag	UNP A0A565A192
A	115	GLN	-	expression tag	UNP A0A565A192
A	116	ALA	-	expression tag	UNP A0A565A192
A	182	ALA	THR	engineered mutation	UNP A0A565A192
A	354	ALA	SER	engineered mutation	UNP A0A565A192
A	382	LEU	-	expression tag	UNP A0A565A192
A	383	GLU	-	expression tag	UNP A0A565A192
A	384	ASN	-	expression tag	UNP A0A565A192
A	385	LEU	-	expression tag	UNP A0A565A192
A	386	TYR	-	expression tag	UNP A0A565A192
A	387	PHE	-	expression tag	UNP A0A565A192
A	388	GLN	-	expression tag	UNP A0A565A192
B	113	GLY	-	expression tag	UNP A0A565A192
B	114	THR	-	expression tag	UNP A0A565A192
B	115	GLN	-	expression tag	UNP A0A565A192
B	116	ALA	-	expression tag	UNP A0A565A192
B	182	ALA	THR	engineered mutation	UNP A0A565A192
B	354	ALA	SER	engineered mutation	UNP A0A565A192
B	382	LEU	-	expression tag	UNP A0A565A192
B	383	GLU	-	expression tag	UNP A0A565A192
B	384	ASN	-	expression tag	UNP A0A565A192
B	385	LEU	-	expression tag	UNP A0A565A192

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Chain	Residue	Modelled	Actual	Comment	Reference
B	386	TYR	-	expression tag	UNP A0A565A192
B	387	PHE	-	expression tag	UNP A0A565A192
B	388	GLN	-	expression tag	UNP A0A565A192
D	113	GLY	-	expression tag	UNP A0A565A192
D	114	THR	-	expression tag	UNP A0A565A192
D	115	GLN	-	expression tag	UNP A0A565A192
D	116	ALA	-	expression tag	UNP A0A565A192
D	182	ALA	THR	engineered mutation	UNP A0A565A192
D	354	ALA	SER	engineered mutation	UNP A0A565A192
D	382	LEU	-	expression tag	UNP A0A565A192
D	383	GLU	-	expression tag	UNP A0A565A192
D	384	ASN	-	expression tag	UNP A0A565A192
D	385	LEU	-	expression tag	UNP A0A565A192
D	386	TYR	-	expression tag	UNP A0A565A192
D	387	PHE	-	expression tag	UNP A0A565A192
D	388	GLN	-	expression tag	UNP A0A565A192

- Molecule 2 is a protein called Nanobody D7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	118	Total	C	N	O	S	0	0	0
			922	583	157	178	4			
2	C	122	Total	C	N	O	S	0	0	0
			954	601	165	184	4			
2	F	122	Total	C	N	O	S	0	0	0
			954	601	165	184	4			

- Molecule 3 is a protein called Thrombospondin-related apical membrane protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	13	Total	C	N	O	S	0	0	0
			91	58	14	18	1			
3	H	13	Total	C	N	O	S	0	0	0
			98	64	14	19	1			
3	I	12	Total	C	N	O	S	0	0	0
			86	55	13	17	1			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	19	GLY	-	expression tag	UNP A0A565A3Y0
G	20	THR	-	expression tag	UNP A0A565A3Y0

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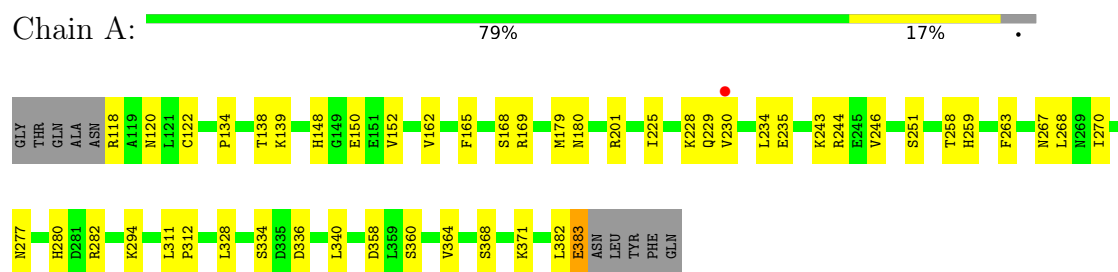
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Chain	Residue	Modelled	Actual	Comment	Reference
G	117	ALA	SER	engineered mutation	UNP A0A565A3Y0
H	19	GLY	-	expression tag	UNP A0A565A3Y0
H	20	THR	-	expression tag	UNP A0A565A3Y0
H	117	ALA	SER	engineered mutation	UNP A0A565A3Y0
I	19	GLY	-	expression tag	UNP A0A565A3Y0
I	20	THR	-	expression tag	UNP A0A565A3Y0
I	117	ALA	SER	engineered mutation	UNP A0A565A3Y0

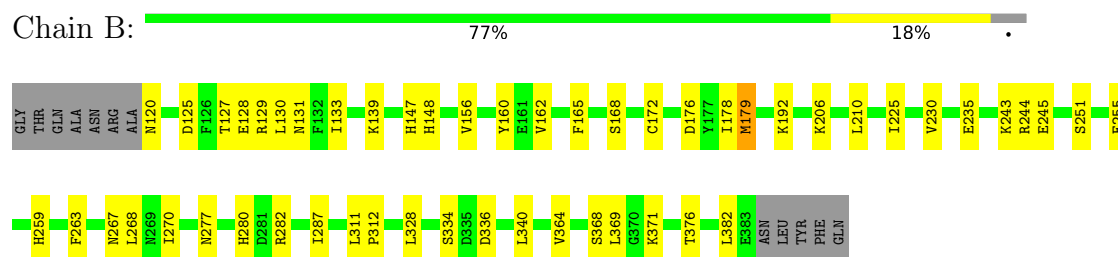
3 Residue-property plots [i](#)

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.

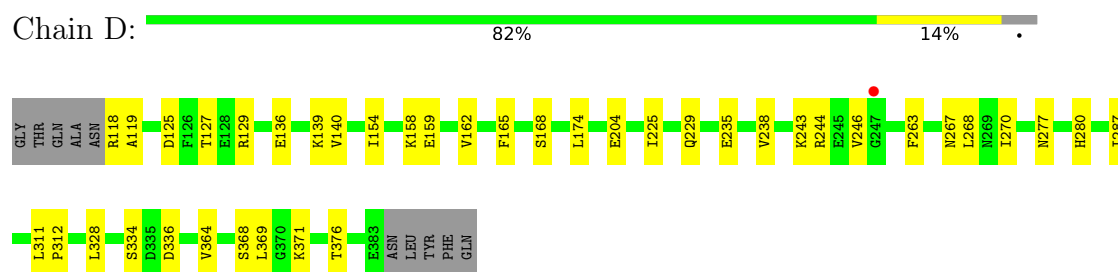
- Molecule 1: Cysteine-rich small secreted protein CSS, putative



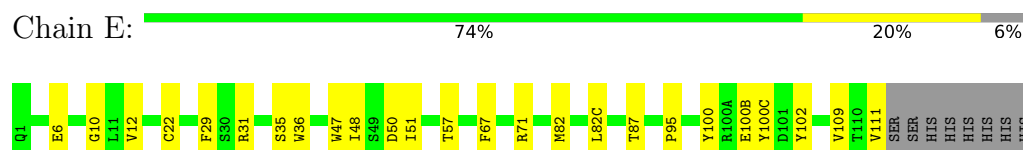
- Molecule 1: Cysteine-rich small secreted protein CSS, putative



- Molecule 1: Cysteine-rich small secreted protein CSS, putative



- Molecule 2: Nanobody D7

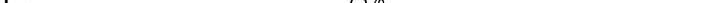


- Molecule 2: Nanobody D7

Chain C:  72% 25%

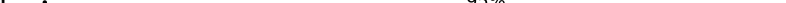


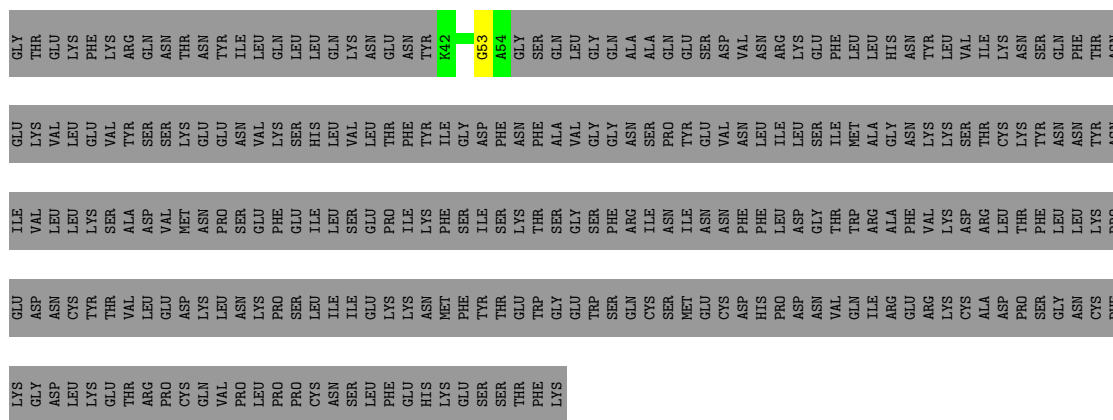
- Molecule 2: Nanobody D7

Chain F:  73% 23% ..

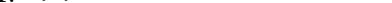


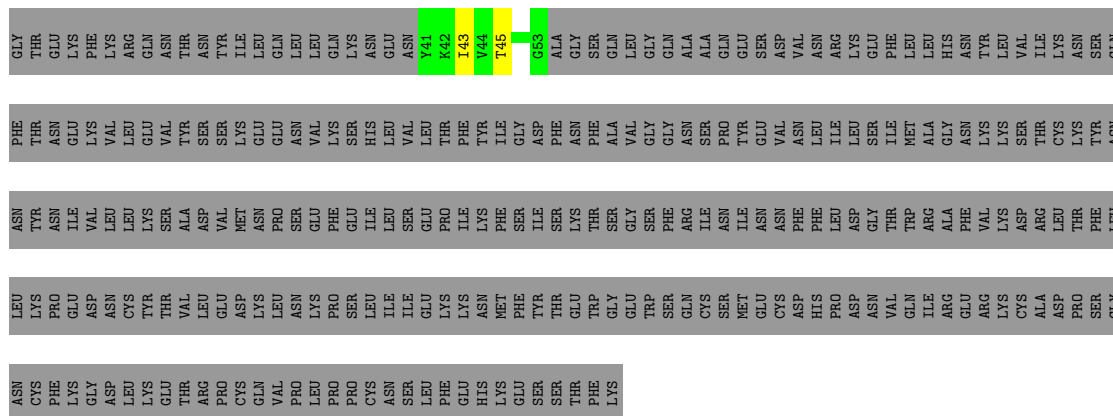
- Molecule 3: Thrombospondin-related apical membrane protein

Chain G:  95%



- Molecule 3: Thrombospondin-related apical membrane protein

Chain H:  95%



- Molecule 3: Thrombospondin-related apical membrane protein

Chain I: ..

96%

SER	PHE	TYR	SER	GLY
GLY	LEU	ASN	GLN	THR
ASN	LEU	ASN	PHE	GLU
CYS	LYS	TYR	THR	LYS
PHE	PRO	ASN	ASN	PHE
LYS	GLU	ILE	GLU	LYS
GLY	ASP	VAL	LYS	ARG
ASP	ASN	LEU	VAL	GLN
LEU	CYS	LEU	LEU	ASN
LYS	TYR	LYS	GLU	THR
GLU	THR	SER	VAL	ASN
THR	VAL	ALA	TYR	TYR
ARG	LEU	ASP	SER	ILE
PRO	GLU	VAL	SER	GLN
CYS	ASP	MET	LYS	LEU
GLN	LYS	ASN	GLU	LEU
VAL	LEU	PRO	GLU	LEU
PRO	ASN	SER	ASN	GLN
LEU	LYS	GLU	VAL	LYS
PRO	PRO	PHE	LYS	ASN
PRO	SER	GLU	SER	GLU
CYS	LEU	ILE	HIS	ASN
ASN	ILE	LEU	LEU	TYR
SER	ILE	SER	VAL	K42
LEU	GLU	GLU	LEU	V43
PHE	LYS	PRO	THR	V44
GLU	LYS	ILE	PHE	V45
HIS	LYS	LYS	TVR	L46
LYS	MET	PHE	ILE	E47
GLU	PHE	SER	GLY	G53
SER	TYR	ILE	ASP	ALA
SER	THR	SER	PHE	GLY
THR	GLU	LYS	ASN	SER
PHE	TRP	THR	PHE	SER
LYS	GLY	SER	ALA	GLN
	GLU	GLY	VAL	LEU
	TRP	SER	GLY	GLY
	SER	PHE	GLY	GLN
	GLN	ARG	ASN	ALA
	CYS	ILE	SER	ALA
	CYS	ASN	PRO	GLN
	MET	ILE	TYR	GLU
	GLU	ASN	GLU	SER
	ASP	ASN	VAL	ASP
	ASP	PHE	ASN	VAL
	HIS	PHE	LEU	ASN
	PRO	LEU	ILE	ARG
	ASP	ASP	LEU	LYS
	ASN	GLY	SER	GLU
	VAL	THR	ILE	PHE
	GLN	TRP	MET	LEU
	ILE	ARG	ALA	LEU
	ARG	ALA	GLY	HIS
	GLU	PHE	ASN	ASN
	ARG	VAL	LYS	TYR
	LYS	LYS	VAL	LEU
	CYS	ASP	SER	VAL
	ALA	ARG	THR	ILE
	ASP	LEU	CYS	LYS
	PRO	THR	LYS	ASN

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	125.22Å 125.22Å 106.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.32 – 3.14 48.32 – 3.14	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.32-3.14) 99.9 (48.32-3.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.225 , 0.273 0.224 , 0.271	Depositor DCC
R_{free} test set	1700 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å ²)	97.5	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 67.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l 0.046 for h,-h-k,-l 0.087 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9548	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.14	0/2201	0.39	0/2976
1	B	0.16	0/2185	0.40	0/2955
1	D	0.15	0/2201	0.36	0/2976
2	C	0.15	0/979	0.43	0/1325
2	E	0.13	0/945	0.38	1/1279 (0.1%)
2	F	0.14	0/979	0.40	0/1325
3	G	0.10	0/91	0.33	0/123
3	H	0.14	0/99	0.31	0/134
3	I	0.32	0/86	0.52	0/116
All	All	0.15	0/9766	0.39	1/13209 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	10	GLY	N-CA-C	6.34	117.97	111.56

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	2153	0	2107	31	0
1	B	2137	0	2089	31	0
1	D	2153	0	2107	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	954	0	898	22	0
2	E	922	0	874	16	0
2	F	954	0	898	20	0
3	G	91	0	95	1	0
3	H	98	0	99	2	0
3	I	86	0	90	3	0
All	All	9548	0	9257	137	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 (137) 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:F:9:GLY:HA2	2:F:18:LEU:HD21	1.61	0.81
2:C:12:VAL:HG11	2:C:82(C):LEU:HD22	1.66	0.77
2:C:39:GLN:HB2	2:C:45:LEU:HD23	1.67	0.75
2:F:37:VAL:HG12	2:F:47:TRP:HA	1.68	0.74
1:B:128:GLU:OE2	1:B:131:ASN:ND2	2.23	0.72
1:A:118:ARG:N	3:I:53:GLY:O	2.27	0.68
1:B:139:LYS:HA	1:B:235:GLU:O	1.91	0.68
1:A:244:ARG:HD3	1:A:267:ASN:HA	1.75	0.68
1:A:243:LYS:NZ	1:A:277:ASN:OD1	2.27	0.68
1:D:118:ARG:NH1	1:D:119:ALA:O	2.28	0.67
3:G:53:GLY:O	1:B:120:ASN:N	2.29	0.65
1:A:165:PHE:N	1:A:168:SER:OG	2.30	0.63
2:C:84:PRO:HA	2:C:111:VAL:HB	1.81	0.63
1:B:156:VAL:HG13	1:B:206:LYS:HB2	1.81	0.63
1:B:162:VAL:HG22	1:B:225:ILE:HG23	1.81	0.62
1:A:148:HIS:CE1	1:A:244:ARG:HG2	2.34	0.62
3:H:43:ILE:HG13	1:D:136:GLU:HB2	1.82	0.61
1:D:364:VAL:HB	1:D:368:SER:HB2	1.83	0.60
2:C:9:GLY:HA2	2:C:18:LEU:HD21	1.84	0.60
2:F:10:GLY:HA2	2:F:109:VAL:HA	1.86	0.58
2:F:47:TRP:NE1	2:F:50:ASP:OD1	2.36	0.57
1:A:138:THR:HG22	3:I:43:ILE:HB	1.85	0.57
2:F:47:TRP:CD1	2:F:100(C):TYR:HH	2.23	0.56
2:C:96:GLN:NE2	2:C:101:ASP:OD1	2.33	0.56
2:F:88:ALA:HB3	2:F:90:TYR:HE1	1.70	0.56
2:C:2:VAL:HG11	2:C:102:TYR:CG	2.41	0.55
1:A:228:LYS:HG2	1:A:229:GLN:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:87:THR:HG23	2:C:110:THR:HG22	1.89	0.55
1:D:162:VAL:HG22	1:D:225:ILE:HG23	1.88	0.54
1:A:258:THR:OG1	1:A:294:LYS:NZ	2.41	0.54
1:D:174:LEU:HD13	1:D:369:LEU:HG	1.91	0.53
1:A:122:CYS:O	1:A:152:VAL:HA	2.09	0.53
2:F:87:THR:HG23	2:F:110:THR:HA	1.92	0.53
2:F:31:ARG:HD2	1:D:246:VAL:HA	1.91	0.52
1:B:125:ASP:OD1	1:B:127:THR:OG1	2.19	0.52
1:A:364:VAL:HB	1:A:368:SER:HB2	1.90	0.52
1:A:277:ASN:HD22	1:A:282:ARG:NH1	2.07	0.52
2:C:6:GLU:OE1	2:C:6:GLU:N	2.42	0.52
2:C:47:TRP:HH2	2:C:50:ASP:HB3	1.75	0.52
1:A:120:ASN:HB2	1:A:150:GLU:HG2	1.90	0.52
2:E:12:VAL:HG11	2:E:82(C):LEU:HD12	1.93	0.51
1:B:243:LYS:NZ	1:B:277:ASN:OD1	2.44	0.51
1:D:243:LYS:NZ	1:D:277:ASN:OD1	2.45	0.50
1:B:334:SER:C	1:B:336:ASP:H	2.19	0.50
2:E:35:SER:HB3	2:E:50:ASP:HB3	1.92	0.50
2:C:2:VAL:HG21	2:C:102:TYR:CE2	2.47	0.50
1:D:270:ILE:HA	1:D:371:LYS:HB2	1.94	0.50
1:B:148:HIS:CE1	1:B:244:ARG:HG2	2.48	0.49
1:B:270:ILE:HA	1:B:371:LYS:HB2	1.94	0.49
1:B:311:LEU:HB3	1:B:312:PRO:HD3	1.93	0.49
1:D:158:LYS:HE3	1:D:204:GLU:HB2	1.94	0.49
2:E:95:PRO:HA	2:E:100(C):TYR:HD1	1.77	0.49
2:F:2:VAL:HG11	2:F:102:TYR:CD2	2.48	0.48
1:B:282:ARG:HH12	1:B:369:LEU:HB3	1.78	0.48
2:F:94:LYS:NZ	1:D:280:HIS:HB2	2.29	0.48
1:A:139:LYS:HA	1:A:235:GLU:O	2.13	0.48
2:F:6:GLU:HA	2:F:22:CYS:HA	1.96	0.48
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.96	0.48
2:F:102:TYR:CE2	1:D:280:HIS:HB3	2.49	0.47
2:E:100:TYR:CE2	2:E:100(B):GLU:HB2	2.50	0.47
1:A:334:SER:C	1:A:336:ASP:H	2.21	0.47
2:C:95:PRO:O	2:C:97:ALA:N	2.42	0.47
1:A:246:VAL:HA	2:E:31:ARG:HD2	1.97	0.47
2:C:11:LEU:HD12	2:C:11:LEU:O	2.14	0.47
2:C:102:TYR:CE2	1:B:280:HIS:HB3	2.50	0.47
1:B:311:LEU:HD13	1:B:340:LEU:HD22	1.97	0.47
2:E:6:GLU:HA	2:E:22:CYS:HA	1.96	0.46
2:E:36:TRP:O	2:E:48:ILE:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:6:GLU:OE1	2:F:6:GLU:N	2.40	0.46
2:C:36:TRP:O	2:C:48:ILE:HB	2.16	0.46
2:F:101:ASP:OD1	2:F:101:ASP:N	2.40	0.46
2:C:102:TYR:HE2	1:B:280:HIS:HB3	1.81	0.46
2:F:84:PRO:HA	2:F:111:VAL:HB	1.97	0.46
2:C:13:GLN:HB3	2:C:115:HIS:NE2	2.31	0.45
2:F:6:GLU:CD	2:F:106:GLY:H	2.24	0.45
2:F:48:ILE:HG23	2:F:63:VAL:HG21	1.99	0.45
1:B:282:ARG:NH1	1:B:369:LEU:HB3	2.31	0.45
1:D:287:ILE:HD13	1:D:376:THR:HB	1.99	0.45
1:A:251:SER:HB2	1:A:259:HIS:HB3	1.99	0.45
1:A:270:ILE:HA	1:A:371:LYS:HB2	1.99	0.45
1:B:156:VAL:HG23	1:B:160:TYR:HD2	1.81	0.45
1:D:154:ILE:HD13	1:D:238:VAL:HG21	1.99	0.45
1:A:134:PRO:HG3	1:A:234:LEU:HB2	1.99	0.45
1:B:172:CYS:O	1:B:176:ASP:N	2.50	0.45
1:B:192:LYS:O	1:B:210:LEU:HD12	2.17	0.45
1:A:311:LEU:HD11	1:A:328:LEU:HD21	1.99	0.44
2:E:51:ILE:HG13	2:E:57:THR:HG22	1.99	0.44
1:D:311:LEU:HB3	1:D:312:PRO:HD3	1.98	0.44
1:A:169:ARG:HD2	1:A:180:ASN:OD1	2.17	0.44
2:F:82:MET:HE2	2:F:82(C):LEU:HD11	2.00	0.44
1:D:334:SER:C	1:D:336:ASP:H	2.25	0.44
1:A:280:HIS:HB3	2:E:102:TYR:CE2	2.53	0.44
2:C:82(C):LEU:HB3	2:C:111:VAL:HG21	2.00	0.44
1:B:263:PHE:HA	1:B:268:LEU:O	2.18	0.44
1:A:263:PHE:HA	1:A:268:LEU:O	2.18	0.44
1:D:311:LEU:HD11	1:D:328:LEU:HD21	2.00	0.44
1:B:179:MET:HE2	1:B:179:MET:HB3	1.95	0.44
1:D:263:PHE:HA	1:D:268:LEU:O	2.18	0.43
2:E:67:PHE:CZ	2:E:82:MET:HE3	2.53	0.43
1:A:358:ASP:OD1	1:A:360:SER:OG	2.35	0.43
1:D:165:PHE:N	1:D:168:SER:OG	2.47	0.43
1:A:162:VAL:HG22	1:A:225:ILE:HG23	2.00	0.43
2:E:87:THR:HG23	2:E:109:VAL:O	2.19	0.43
1:D:244:ARG:HD3	1:D:267:ASN:HA	2.01	0.43
1:A:382:LEU:O	1:A:383:GLU:C	2.61	0.43
2:E:12:VAL:O	2:E:111:VAL:HA	2.19	0.42
2:F:39:GLN:NE2	2:F:43:LYS:O	2.36	0.42
1:B:147:HIS:NE2	1:B:245:GLU:HG2	2.34	0.42
1:B:311:LEU:HD11	1:B:328:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:VAL:HB	1:B:368:SER:HB2	2.01	0.42
1:B:130:LEU:HB2	1:B:160:TYR:CE2	2.54	0.42
1:A:228:LYS:HE3	1:A:229:GLN:HG2	2.01	0.42
1:D:159:GLU:HB3	1:D:229:GLN:NE2	2.34	0.42
1:B:133:ILE:HG12	1:B:230:VAL:HG11	2.01	0.42
1:A:228:LYS:O	1:A:230:VAL:HG23	2.19	0.41
1:B:165:PHE:N	1:B:168:SER:OG	2.52	0.41
2:E:47:TRP:HH2	2:E:50:ASP:HB3	1.84	0.41
2:C:13:GLN:CD	2:C:13:GLN:H	2.28	0.41
2:C:20:LEU:O	2:C:79:TYR:HA	2.19	0.41
1:A:311:LEU:HD13	1:A:340:LEU:HD22	2.03	0.41
2:C:10:GLY:N	2:C:108:GLN:O	2.53	0.41
2:F:90:TYR:O	2:F:106:GLY:HA2	2.21	0.41
2:E:29:PHE:O	2:E:71:ARG:NH2	2.54	0.41
2:C:87:THR:HG23	2:C:110:THR:HA	2.02	0.41
1:B:287:ILE:HD13	1:B:376:THR:HB	2.02	0.41
3:I:47:GLU:HG2	3:I:47:GLU:O	2.21	0.41
2:E:82:MET:HB3	2:E:82(C):LEU:HD21	2.03	0.41
2:C:14:PRO:HD3	2:C:112:SER:O	2.20	0.41
1:B:255:GLU:H	1:B:255:GLU:CD	2.29	0.41
1:D:125:ASP:OD1	1:D:127:THR:OG1	2.23	0.40
1:D:139:LYS:HA	1:D:235:GLU:O	2.20	0.40
1:A:169:ARG:HA	1:A:179:MET:O	2.22	0.40
2:E:48:ILE:HD13	2:E:48:ILE:HA	1.89	0.40
3:H:45:THR:HB	1:D:140:VAL:HA	2.02	0.40
1:B:251:SER:HB2	1:B:259:HIS:HB3	2.03	0.40
1:B:244:ARG:HD3	1:B:267:ASN:HA	2.03	0.40
1:A:201:ARG:HE	1:A:201:ARG:HB2	1.78	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	264/276 (96%)	244 (92%)	20 (8%)	0	100	100
1	B	262/276 (95%)	240 (92%)	22 (8%)	0	100	100
1	D	264/276 (96%)	244 (92%)	20 (8%)	0	100	100
2	C	120/126 (95%)	110 (92%)	10 (8%)	0	100	100
2	E	116/126 (92%)	110 (95%)	6 (5%)	0	100	100
2	F	120/126 (95%)	109 (91%)	11 (9%)	0	100	100
3	G	11/279 (4%)	10 (91%)	1 (9%)	0	100	100
3	H	11/279 (4%)	10 (91%)	1 (9%)	0	100	100
3	I	10/279 (4%)	9 (90%)	1 (10%)	0	100	100
All	All	1178/2043 (58%)	1086 (92%)	92 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	248/256 (97%)	247 (100%)	1 (0%)	84	84
1	B	247/256 (96%)	243 (98%)	4 (2%)	55	71
1	D	248/256 (97%)	247 (100%)	1 (0%)	84	84
2	C	99/103 (96%)	98 (99%)	1 (1%)	68	76
2	E	95/103 (92%)	95 (100%)	0	100	100
2	F	99/103 (96%)	96 (97%)	3 (3%)	36	61
3	G	10/257 (4%)	10 (100%)	0	100	100
3	H	11/257 (4%)	11 (100%)	0	100	100
3	I	10/257 (4%)	9 (90%)	1 (10%)	7	25
All	All	1067/1848 (58%)	1056 (99%)	11 (1%)	68	76

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	383	GLU
2	C	114	HIS
2	F	101	ASP
2	F	114	HIS
2	F	115	HIS
1	B	129	ARG
1	B	178	ILE
1	B	179	MET
1	B	382	LEU
1	D	129	ARG
3	I	45	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	GLN
1	A	350	ASN
2	C	81	GLN
2	C	82(A)	ASN
2	F	108	GLN
1	B	249	GLN
1	B	267	ASN
1	B	293	ASN
1	D	200	HIS
1	D	211	GLN
1	D	249	GLN
1	D	293	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	266/276 (96%)	-0.22	1 (0%) 88 76	62, 89, 127, 162	0
1	B	264/276 (95%)	-0.21	0 100 100	45, 73, 133, 174	0
1	D	266/276 (96%)	-0.18	1 (0%) 88 76	60, 84, 125, 146	0
2	C	122/126 (96%)	-0.18	0 100 100	51, 94, 143, 169	0
2	E	118/126 (93%)	0.05	0 100 100	71, 122, 160, 173	0
2	F	122/126 (96%)	-0.14	0 100 100	60, 96, 132, 172	0
3	G	13/279 (4%)	0.50	0 100 100	103, 110, 123, 133	0
3	H	13/279 (4%)	0.55	0 100 100	86, 100, 115, 120	0
3	I	12/279 (4%)	0.85	1 (8%) 17 9	87, 115, 120, 126	0
All	All	1196/2043 (58%)	-0.14	3 (0%) 90 80	45, 90, 140, 174	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	53	GLY	2.3
1	A	230	VAL	2.2
1	D	247	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.